The INTERNATIONAL CONFERENCE on
APPLIED MATHEMATICS,
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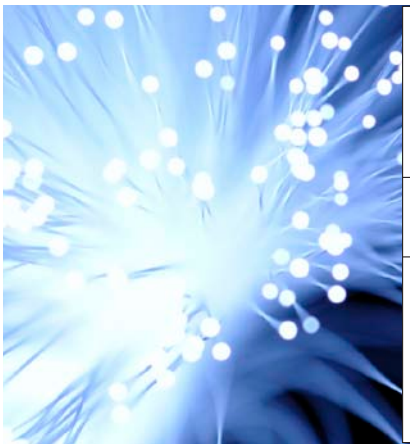

AMMCS2011

A Laurier Centennial Conference

JULY 25–29

WILFRID LAURIER UNIVERSITY | WATERLOO, ONTARIO, CANADA

BOOK OF ABSTRACTS

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BOOK OF ABSTRACTS:

THE INTERNATIONAL CONFERENCE ON APPLIED MATHEMATICS, MODELING AND COMPUTATIONAL SCIENCE

WATERLOO, CANADA, JULY 25 - 29, 2011

LAURIER CENTENNIAL CONFERENCE: AMMCS-2011

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Publisher: AMMCS@2011
ISBN: 2810000004711

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SS-SND	Symmetry in Nonlinear Dynamics: Applications and Numerics	Pietro-Luciano Buono, *UOIT (Canada)* Manuele Santoprete, *Wilfrid Laurier University (Canada)* Cristina Stoica, *Wilfrid Laurier University (Canada)*
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SS-TAF	Theory and Applications in Finance	Joe Campolieti, *Wilfrid Laurier University (Canada)* Nick Costanzino, *Wilfrid Laurier University (Canada)* Roman Makarov, *Wilfrid Laurier University (Canada)*
SS-VS	Numerical Methods for First and Second Order Fully Nonlinear PDEs	Xiaobing Feng, *University of Tennessee (USA)* Chiu-Yen Kao, *The Ohio State University (USA)* Ying Wang, *University of Minnesota (USA)*

CS Code	Contributed Session Title	Session Chairs
CS-MECHE	Computational Mechanics and Engineering	Sanjay Prabhakar, *Wilfrid Laurier University (Canada)* Rakesh Dhote, *University of Toronto (Canada)*
CS-MODELING	Partial Differential and Integral Equations in Mathematical Modeling	Yulia Gel, *University of Waterloo (Canada)* Kimberly Levere, *University of Guelph (Canada)* Sanjay Prabhakar, *Wilfrid Laurier University (Canada)*
CS-DSDE	Applications of Dynamical Systems and Differential Equations	Ilias Kotsireas, *Wilfrid Laurier University (Canada)* Danielle Alessio, *Wilfrid Laurier University (Canada)*
CS-BSM	Mathematics and Computation in Biological Sciences and Medicine	Alex Zhukov, *Wilfrid Laurier University (Canada)*
CS-CPC	Computational Physics and Chemistry	Brian West, *Wilfrid Laurier University (Canada)* Steven Burger, *McMaster University (Canada)*
CS-CACO	Computational Algebra, Combinatorics and Optimization	Hongbing Fan, *Wilfrid Laurier University (Canada)* Yuzhen Xie, *University of Western Ontario (Canada)*
CS-POSTER	AMMCS-2011 Poster Session	
CS-ENVIRONMENT	Mathematical Modeling in Environmental Sciences and Models for Complex Media	Rakesh Dhote, *University of Toronto (Canada)*
CS-APMRE	Applied Problems and Methods in Research & Education	Douglas Woolford, *Wilfrid Laurier University (Canada)*
CS-FINANCE	Financial Mathematics and Computation	Roman Makarov, *Wilfrid Laurier University (Canada)* Y. George Lai, *Wilfrid Laurier University (Canada)*

PLENARY AND SEMI-PLENARY SESSIONS

AMMCS-2011, Laurier Centennial:
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Stephen Watt

Computer Science Department, The University of Western Ontario (Canada)

Stephen Watt is Distinguished University Professor of the University of Western Ontario, located in London, Canada. He received his PhD from the University of Waterloo in 1986 for early work on parallel computer algebra. Watt held a series of positions at IBM Research at Yorktown Heights, then the University of Nice and INRIA, before arriving at the University of Western Ontario in 1997. Watt is internationally recognized as an expert in the field of computer algebra. He was one of the early investigators in parallel computer algebra systems and a pioneer in the areas of symbolic-numeric algorithms and mathematical knowledge management. He is one of the original authors of the Maple and Axiom computer algebra systems, creator of the Aldor programming language for symbolic computation and a principal in the creation of the MathML and InkML internet standards. His current areas of focus are algorithms for polynomials with symbolic exponents and mathematical handwriting recognition.

Mathematical Modeling in Mathematical Handwriting Recognition

Accurate computer recognition of handwritten mathematics offers to provide a natural interface for mathematical computing, document creation and collaboration. Mathematical handwriting, however, provides a number of challenges beyond what is required for the recognition of handwritten natural languages. On one hand, it is usual to use symbols from a range of different alphabets and there are many similar-looking symbols. Mathematical notation is two-dimensional and size and placement information is important. Additionally, there is no fixed vocabulary of mathematical "words" that can be used to disambiguate symbol sequences. On the other hand there are some simplifications. For example, symbols do tend to be well segmented. With these characteristics, new methods of character recognition are important for accurate handwritten mathematics input.

We present a geometric theory that we have found useful for recognizing mathematical symbols. Characters are represented as parametric curves approximated by certain truncated orthogonal series. This maps symbols to a low dimensional vector space of series coefficients in which the Euclidean distance is closely related to the variational integral between two curves. This can be used to find similar symbols very efficiently. We describe some properties of mathematical handwriting data sets when mapped into this space and compare classification methods and their confidence measures. We also show how, by choosing the functional basis appropriately, the series coefficients can be computed in real-time, as the symbol is being written and, by using integral invariant functions, orientation-independent recognition is achieved. The beauty of this theory is that a single, coherent view provides several related geometric techniques that give a high recognition rate and that do not rely on peculiarities of the symbol set.

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Igor Shparlinski

Department of Computing, Macquarie University (Australia)

Igor Shparlinski is a Professor of Macquarie University, in 2010 he was awarded the title of Distinguished Professor. In 1996, he was awarded a Medal of the Australian Mathematical Society for his activities in the area of applications of number theory to computer science. He is a fellow of the Australian Academy of Science (since 2006) and of the Australian Mathematical Society (since 2000). He is a recipient of Australian Professorial Fellowship (2005-2010) and the Medal of the Australian Mathematical Society.

His research areas are number theory and its applications to computer science, cryptography and discrete mathematics. He serves on editorial boards of several journals specialising in these areas.

Group Structures of Elliptic Curves: Statistics, Heuristics, Algorithms

We study the collection of group structures that can be realized as a group of rational points on an elliptic curve over a finite field (such groups are well known to be of rank at most two). We also study various subsets of this collection.

Some of these results are rigorous and based on recent advances in analytic number theory, some are conditional under certain widely believed conjectures, and others are purely heuristic in nature and exhibit several interesting and unexplained phenomena in the distribution of group structures.

Finally, we discuss some algorithms to compute group structures of elliptic curves over finite fields.

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David Cai

Courant Institute, New York University (USA)

David Cai is currently a professor of mathematics and neural science at Courant Institute of Mathematical Sciences and the Center for Neural Science, New York University. He received his B.S. from Peking University, China, and Ph.D. from Northwestern University, U.S. His research interests include applied mathematics, theoretical physics, and theoretical and computational neuroscience

Mathematical Analysis of Neuronal Network Dynamics

From the perspective of nonlinear dynamical systems, nonequilibrium statistical physics, and scientific modeling, we will review our computational modeling of the dynamics of the primary visual cortex and describe recent developments of mathematical methods used in analysis of the dynamics of neuronal networks arising from the brain.

We will present a kinetic theory approach to study neuronal network dynamics and discuss the interplay between the dynamics over the network and the topology of the network, such as random networks and scale-free networks. Finally we will briefly address the issue of anatomical connectivity and functional connectivity in the brain.

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Mark Carpenter

NASA Langley Research Center (USA)

Mark H. Carpenter received a BS in Chemistry from Bethel College in 1981, and a PhD in Mechanical Engineering (combustion emphasis) from Carnegie-Mellon in 1986. After graduation he accepted a position at NASA Langley Research Center, Hampton VA, USA. He has worked at Langley continuously for nearly 25 years, with the exception of a sabbatical year (2006) serving as a visiting professor at "Technical University of Delft", Delft, The Netherlands. His research interests include the development of 1) high-order finite difference and spectral methods, 2) high-order explicit and implicit temporal integrators and 3) linear and nonlinear solvers. The applications motivating this development over the past decade include DNS/LES of high-speed, chemically reacting flows, boundary layer stability and transition phenomena, and acoustic liner development. He currently serves on the editorial board of Journal of Scientific Computing, and the advisory panel for the International Conference of Spectral and High-order methods.

Towards a Robust, Multi-Domain, Energy Stable WENO Formulation for High Speed Flows

Weighted Essentially NonOscillatory (WENO) schemes are routinely used to perform high resolution simulations of canonical problems containing discontinuities, and are extremely successful in this context. Because conventional WENO formulations have numerous structural and design constraints (e.g. structured meshes, accuracy, conservation, stencil biasing...), extension to complex geometries is problematic. Herein, we demonstrate a general multi-block WENO capability, based on uniformly accurate fourth-order and sixth-order, finite-domain, Energy Stable WENO (ESWENO) operators. The individual blocks feature boundary closures that maintain design accuracy, conservation and L^2 stability, while accommodating full WENO stencil biasing. The adjoining blocks are coupled using interface penalties motivated by Internal Penalty and DG formulations. Test cases are presented that demonstrate the efficacy of the new multi-domain ESWENO approach on high speed flow problems.

This work is performed in conjunction with Dr. Nail K. Yamaleev (North Carolina A&T State University, USA), and Travis Fisher (NASA Langley Research Center, USA).

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Walter Craig

Department of Mathematics and Statistics McMaster University (Canada)

Dr. Craig received his doctorate in mathematics in 1981 from the Courant Institute. Following this he has held academic positions in the California Institute of Technology, Stanford University and Brown University, where he was chair of the Mathematics Department. He moved to McMaster University in 2000 as Canada Research Chair of Mathematical Analysis and its Applications. His research interests are in nonlinear partial differential equation, Hamiltonian dynamical systems, and their applications to problems motivated by the physical sciences. He has been a Sloan Foundation Fellow, and he is currently a Killam Research Fellow. He was elected to the Royal Society of Canada in 2007.

Lower Bounds on the Navier-Stokes Singular Set

The well-known result of partial regularity for solutions of the Navier-Stokes equations provides an upper bound on the size of the singular set of (suitable) weak solutions. This talk will describe complementary lower bounds, both for the the singular set and the energy (L2) concentration set, in case that they are nonempty. These bounds are microlocal in nature, and are based on a novel estimate for weak solutions of the Navier-Stokes equations.

Part of these results represents joint work with A. Biryuk and M. Arnold

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Suzanne Lenhart

Mathematics Department, University of Tennessee, Knoxville (USA)

Suzanne Lenhart is a full professor in the Mathematics Department at the University of Tennessee. She was a part-time research staff member at Oak Ridge National Laboratory from 1987-2009. Her research involves partial differential equations, ordinary differential equations and optimal control of biological and physical models. She has a 2007 book, "Optimal Control applied to Biological Models."

She was the President of the Association for Women in Mathematics in 2001-2002. She was elected to the Board of Trustees of the Society for Industrial and Applied Mathematics in 2004 and again in 2007. She is the Associate Director for Education, Outreach and Diversity for the National Institute for Mathematical and Biological Synthesis. Lenhart was the director of the Research Experiences for Undergraduates summer program for UT Math. Dept. from 1990-2005 and now directs such a program for the institute.

Mixing it up: Discrete and Continuous Optimal Control for Biological Models

This presentation will illustrate optimal control methods applied to several types of models, including a mixture of discrete and continuous features. The applications range from a discrete model for cardiopulmonary resuscitation to partial differential equation models for rabies in raccoons. Detailed results will be given for harvesting in a PDE fishery model that answers the question: Does a marine reserve occur when maximizing harvest yield?

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Alan Edelman

Department of Mathematics, Massachusetts Institute of Technology (USA)

Professor Edelman has been working in the area of random matrix theory, numerical algorithms and high performance computing for 25 years. He has won many prizes for his work including the prestigious Householder Award, Gordan Bell Prize, and various Best Paper Prizes. In 2011 he was elected a SIAM Fellow. He is the founder of Interactive Supercomputing acquired by Microsoft. He holds and has applied for several patents in the area of high performance computing networks, algorithms, and software. He is widely recognized for his broad expertise in pure mathematics, algorithms, and applications. Edelman has consulted for IBM, Thinking Machines, Pixar, Akamai, Microsoft, Los Alamos National Labs, and others. Random Matrix Theory is a deep passion. He believes that whole branches of science and engineering are waiting to be transformed by this subject.

Random Matrix Theory in Applied Mathematics, Modeling, and Computational Science

Random matrix theory continues to be a powerful tool for so many applications, yet the number of scientists familiar with the various aspects of the theory remains relatively small at this time. Further the theory is developing rapidly with very many open problems. This talk will give a general overview of the theory and delve into a few applications and open problems.

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Chi-Wang Shu

Division of Applied Mathematics, Brown University (USA)

Chi-Wang Shu obtained his BS degree from the University of Science and Technology of China in 1982 and his PhD degree from the University of California at Los Angeles in 1986. He came to Brown University as an Assistant Professor in 1987, moving up to Associate Professor in 1992 and Full Professor in 1996. He was the Chair of the Division of Applied Mathematics between 1999 and 2005, and is now the Theodore B. Stowell University Professor of Applied Mathematics. His research interest includes high order finite difference, finite element and spectral methods for solving hyperbolic and other convection dominated partial differential equations, with applications to areas such as computational fluid dynamics, semi-conductor device simulations and computational cosmology. He is the managing editor of Mathematics of Computation and the chief editor of Journal of Scientific Computing. His honors include the First Feng Kang Prize of Scientific Computing in 1995 and the SIAM/ACM Prize in Computational Science and Engineering in 2007. He is an ISI Highly Cited Author in Mathematics and a SIAM Fellow.

Inverse Lax-Wendroff Procedure for Numerical Boundary Conditions of Hyperbolic Equations

We develop a high order finite difference numerical boundary condition for solving hyperbolic Hamilton-Jacobi equations and conservation laws on a Cartesian mesh. The challenge results from the wide stencil of the interior high order scheme and the fact that the boundary may not be aligned with the mesh and can intersect the grids in an arbitrary fashion. Our method is based on an inverse Lax-Wendroff procedure for the inflow boundary conditions. We repeatedly use the partial differential equation to write the normal derivatives to the inflow boundary in terms of the tangential derivatives and the time derivatives (for time dependent equations). With these normal derivatives, we can then impose accurate values of ghost points near the boundary by a Taylor expansion. At the outflow boundaries, we use Lagrange extrapolation or least squares extrapolation if the solution is smooth, or a weighted essentially non-oscillatory (WENO) type extrapolation if a shock is close to the boundary. Extensive numerical examples are provided to illustrate that our method is high order accurate and has good performance when applied to one and two dimensional scalar or system cases with the physical boundary not aligned with the grids and with various boundary conditions including the solid wall boundary condition.

This is a joint work with Ling Huang and Mengping Zhang (for the Hamilton-Jacobi equations) and with Sirui Tan (for the time dependent conservation laws).

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Ming Li

David R. Cheriton School of Computer Science, University of Waterloo (Canada)

Ming Li is a Canada Research Chair in Bioinformatics and a University Professor at the University of Waterloo. He is a fellow of the Royal Society of Canada, ACM, and IEEE. He is a recipient of E.W.R. Steacie Fellowship Award in 1996, the 2001 Killam Fellowship, and the 2010 Killam Prize. Together with Paul Vitanyi they have co-authored the book "An Introduction to Kolmogorov Complexity and its Applications". He is a co-managing editor of Journal of Bioinformatics and Computational Biology. He is an Associate Editor-in-Chief of Journal of Computer Science and Technology.

Kolmogorov Complexity and its Applications in Computer Science

Computer Science, as a science of information processing, has risen as a major disclipline during the past half century. Along with it, a new mathematical theory - Kolmogorov complexity - has emerged. In this talk, we will explain two applications of Kolmogorov complexity in computer science.

The first application is on the average-case analysis of algorithms. In computer science, analyzing the average behavior of an algorithm is a difficult task as, by definition, it involves averaging over all inputs. It would make the average-case analysis easy if we could find a "typical input" which causes the program run in the "average-case". Such a typical input can never be found but it exists according to Kolmogorov complexity. We will demonstrate how to use this fact to give an average case analysis of ShellSort, partially solving an open question of 40 years; and to give a very simple proof of Lovasz Local Lemma.

The second application is on how to measure information distance between any two information carrying entities. This optimal metric has been successfully applied to measure the distances between two genomes, two chain letters, two images, two programs, a query and an answer on the internet, and many other applications.

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Alberto Bressan

Department of Mathematics, Penn State University (USA)

Alberto Bressan completed his undergraduate studies at the University of Padova, Italy, and received a Ph.D. from the University of Colorado, Boulder, in 1982. He has held faculty positions at the University of Colorado, Boulder, and at the International School for Advanced Studies in Trieste, Italy. Presently he is Eberly Chair Professor of Mathematics at the Pennsylvania State University.

His scientific interests lie in the areas of differential inclusions, control theory, differential games, and hyperbolic systems of conservation laws.

A. Bressan delivered one of the plenary lectures at the International Congress of Mathematicians, Beijing 2002. He received various awards, including the A. Feltrinelli prize from the Accademia Nazionale dei Lincei in Rome, 2006, and the M. Bôcher prize from the American Mathematical Society, 2008. He currently serves on the editorial board of 17 mathematical journals.

Besides mathematics, he enjoys playing piano and flute. He lives in State College with his wife Wen Shen and two daughters, Luisa Mei and Maria Lan.

Dynamic Blocking Problems

The talk will describe a new class of optimization problems, motivated by the confinement of wild fires, or of the spreading of chemical contaminations. In absence of control, the region burned by the fire is modeled as the reachable set for a differential inclusion. We assume that fire propagation can becontrolled by constructing "barriers", in real time. These are represented by rectifiable sets in the plane, which cannot be crossed by trajectories of the differential inclusion. For this model, several results will be presented, concerning:

1. The speed at which the barrier must be constructed, in order to eventually contain the fire.
2. The existance of an optimal strategy.
3. Relations with Hamilton-Jacobi equations with obstacles.
4. Necessary conditions for optimality, and the "instantaneous value of time".
5. Examples of explicit solutions.

Some related questions and open problems will also be discussed.

SPECIAL SESSIONS AND MINISYMPOSIA

AMMCS-2011

Minisymposium: Applied Analysis & Inverse Problems

SS-AAIP

Organizers:
Marcus Garvie, *University of Guelph (Canada)*
Herb Kunze, *University of Guelph (Canada)*

Inverse problems ask us to recover or estimate information about a mathematical model, given information about a solution. They occur in many branches of science and mathematics. Examples include parameter estimation for ecological systems, physical systems, environmental systems, or economic systems; medical imaging and other imaging applications; and model identification problems in all of these settings. This minisymposium will provide a forum for researchers working on inverse problems to present their ideas. The talks will include aspects of mathematical modeling, applied analysis, and computational methods and algorithms.

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On Level-Set Regularization Methods for Denoising of Binary Images

A. De Cezaro[1] and A. Leitão[2],

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[2] *Department of Mathematics, Federal Univ. of St. Catarina, 88040-900 Florianópolis, Brazil, aleitao@gmail.com*

In this article we investigate regularization methods of level-set type for the inverse problem of denoising of binary images, which is a fundamental problem in image analysis Ref. [1][6][8].

Our first approach is based on the level-set regularization strategy proposed in Ref. [3][4][5]. This method exploits a regularization concept for the solution of ill-posed operator equations, where the operator is composed of a continuous and a discontinuous operator. We generalize the analysis presented in Ref. [3][4][5] with the assumption that the direct operator F is continuous on the spaces $L^p(\Omega)$, $1 \leq p < \infty$. Well-posedness, stability and convergence results of the corresponding Tikhonov functional are proved. In particular, for binary image problems, we provide convergence and stability of the level-set approach in the weak L_2-topology.

A second approach based on a modification of the the Rudin-Osher-Fatemi (ROF) model Ref. [7], is also investigated. We propose a relaxation of the ROF functional, originally defined on the space of binary BV-functions, obtaining a Tikhonov functional defined on the Sobolev space $H^1(\Omega)$ of level-set functions. For this approach we again prove well-posedness of the Tikhonov functional. Moreover, we obtain a relation between the minima of the relaxed functional and the original ROF functional.

The quality of the proposed method is demonstrated by solving the benchmark binary image denoising problem in Ref. [1][6][8].

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Edge Detection as an application of fractal imaging

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Many direct approaches to edge detection have been detailed in the literature. Notably, the Sobel Edge Detector [1] and related approaches by various other researchers approximate gradients in two-dimensional images with the goal of finding curves along which there exists a sharp transition in image values. Second-order derivative approximation methods, such as the edge detector of Marr and Hildrith [2], have provided an alternative direct method. Edge-fitting techniques exist as well.

In fractal image compression, one seeks to approximate a given target image by the fixed point of a contractive operator called the fractal transform. Typically, one uses Local Iterated Function Systems with Grey-Level Maps (LIFSM), where the involved functions map a parent (domain) block in an image to a smaller child (range) block and the grey-level maps adjust the shading of the shrunken block. Iteration of the fractal transform on any initial image produces an approximation of the fixed point and, hence, an approximation of the target image. Since the parameters defining the LIFSM take less space to store than the target image does, image compression is achieved.

We outline a novel edge detection technique that uses ideas from fractal imaging. We introduce some changes to the traditional LIFSM algorithm, allowing for overlapping child blocks and multiple near-optimal parent blocks to be involved in the scheme. The edge detector takes into account two different criteria: the clustering of near-optimal parent blocks, and the values of certain parameters within the algorithm. We show that this indirect approach to edge detection can give results comparable to the well-established edge detection techniques in [1] and [2], for example.

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An Algorithm for Solving Underdetermined Inverse Problem : Application to Pharmacokinetics Model

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As the information we can obtain clinically from a live patient is often much less than the complexity of the internal activity in a patient's body, underdetermined inverse problems appear often in the field of personalized medicine.

In fact, our interest for the underdetermined inverse problem has initiated by the parameter identification problem of a pharmacokinetics model of an anti-cancer drug CPT-11 (also known as Irinotecan). In this problem, we aim to estimate the parameters of the pharmacokinetics model based on the clinically observed data from a patient. The unique aspect of this parameter identification problem is that instead of finding a single set of parameters that is suitable for the pharmacokinetics model to reproduce the clinically observed data, the aim of this problem is to find multiple sets of such parameters. In other word, for underdetermined inverse problems, we often add an extra constraint to make the solution unique; however, we wish to find many solutions of the original underdetermined inverse problem. Although this idea was aimed towards clinical use, due to the lack of accuracy and the unrealistic computational cost, solving this type of inverse problem using conventional algorithm seemed not practical.

Motivated by this example, we have constructed a Newton's method-like algorithm to solve the underdetermined inverse problems. Our iterative scheme starts with a set of widely distributed independent variables. By computing the forward problem at each independent variable, we find a suitable linear approximation of the forward problem in the broad domain where the set of independent variables are distributed. Then by using this linear approximation, we estimate the solutions of this inverse problem and move the set of independent variables accordingly. After few iterations, the set of independent parameters converge and accuracy improvement stagnates. Following their convergence, we use Broyden's method to improve the accuracy by moving each independent parameter separately and achieves the desired accuracy.

Through the numerical experiments of our algorithm compared to other established methods, we have found that our method requires significantly less number of evaluations of the forward problem than the traditional Newton's Method and also far more accurate than the stochastic method. Although our method looks like any other variations of Newton's method, the essential difference is that instead of approximating Jacobian locally, we estimate it more globally using widely distributed independent variables. Owing to this design of the algorithm, we have observed that our method is robust against small "roughness" of the forward simulation compared to a method like Levenberg-Marquardt method. Such roughness appears in the coefficients identification problems of an ODE when the ODE is solved numerically.

Thus we conclude that we have constructed an accurate, robust and computationally efficient algorithm for solving the underdetermined inverse problem of our interest.

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Stability of two IMEX methods, CNLF and BDF2-AB2, for uncoupling systems of evolution equations

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Stability is proven for two second order, two step methods for uncoupling a system of two evolution equations with exactly skew symmetric coupling: the Crank-Nicolson Leap Frog (CNLF) combination and the BDF2-AB2 combination. The form of the coupling studied arises in spatial discretizations of the Stokes-Darcy problem. For CNLF we prove stability for the coupled system under the time step condition suggested by linear stability theory for the Leap-Frog scheme. This seems to be a first proof of a widely believed result. For BDF2-AB2 we prove stability under a condition that is better than the one suggested by linear stability theory for the individual methods.

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A two steps method in inverse scattering problem for a sound-hard crack

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In this paper we consider the inverse problem of reconstructing an unknown sound-hard crack Γ from the measured far field pattern. The mathematical modeling for this problem is the exterior boundary value problem for the Helmholtz equation

$$\Delta u + k^2 u = 0, \quad \text{in } \mathbf{R}^2 \setminus \Gamma \tag{1}$$

with the prescribed Neumann boundary conditions on both sides of the crack.

Based on integral equations approach, this problem was shown in [1] to be equivalent to a two by two system of nonlinear integral equations which were regularized simultaneously because of the ill-posedness of the original inverse problem. One of the drawbacks of this approach is that two regularization parameters are needed to perform the reconstruction. This is remedied in [2] by splitting the problem into two consecutive steps consisting of a forward problem and an ill-posed equation in the case of a sound-soft crack.

In this paper, we will extend the method in [2] to the case of a sound-hard crack. Besides, we will also discuss the reconstruction in the case of limited apperture where data are only measured in some range of angles. Some numeical examples will be given at the end of the paper to demostrate the feasibility of this method.

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A new algorithm for estimating parameters in reaction-diffusion systems that display pattern formation

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We present a new algorithm for estimating parameters in reaction-diffusion systems that display pattern formation via the mechanism of diffusion-driven instability [1]. A Modified Discrete Optimal Control Algorithm (MDOCA) is illustrated with the Schnakenberg [2] and Gierer-Meinhardt [3] reaction-diffusion systems using PDE constrained optimization techniques. The MDOCA algorithm is a modification of a standard variable-step gradient algorithm [4] that yields a huge saving in computational cost. The results of numerical experiments demonstrate that the algorithm accurately estimated key parameters associated with stationary target functions generated from the models themselves. Furthermore, the robustness of the algorithm was verified by performing experiments with target functions perturbed with various levels of additive noise.

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Using the nonlinear Lax-Milgram representation theorem to solve inverse problems for nonlinear reaction-diffusion equations at steady-state

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In recent years there has been great interest in solving inverse problems (with applications in various fields of study). This interest has given rise to an abundance of literature on the subject, and a number of methods for solving inverse problems have been proposed, see for instance [3] and [4]. In this talk we discuss the "collage" based approach to solving inverse problems. In practice, minimizing the approximation error can be a difficult task. The essence of collage based methods is to instead find an upper bound on the approximation error that is more readily minimizable. We extend some of the existing literature on collage based methods (see [1][2]) to the setting of nonlinear problems via the nonlinear Lax-Milgram representation theorem. Necessary background theory will be discussed and the nonlinear generalized collage theorem will be developed. Finally, we will apply this method to a steady-state nonlinear reaction-diffusion model, discuss numerical considerations, and present our results.

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Inverse Problems in Finite and Infinite Dimensional Spaces with Applications in Biomathematics

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In recent years, a variety of "collage theorem"-based frameworks have been developed to solve inverse problems in different settings. The root idea borrows from the tools and the philosophy at the heart of fractal imaging, where one approximates a "target image" by the fixed point of a fractal transform. In solution frameworks for inverse problems in ODEs, PDEs, and integral equations, the idea is to approximate a "target solution" (perhaps in the form of observational data) by the fixed point of a operator or the solution of an operator equation.

In this talk, we recap some past result and present a new framework for solving inverse problems for ODEs in Banach spaces. We contextualize the work by presenting examples linked to recent work/publications in biomathematics:

- A two-stage model of mRNA and protein concentration [2]. The system of ODEs modeling the concentrations features an environmental input that is assumed to be a Markov process switching between two states. The goal of the inverse problem is to recover the decay rates and the mRNA-to-protein translation rate from the observation of numerous realizations of the stochastic process.
- The pathogenesis mechanism of the opportunistic human pathogen *Pseudomonas aeruginosa* in co-culture with *Dictyostelium* amoebae [1]. The dynamics of the interactions feature amoeba feeding on bacteria and bacteria exerting their pathogenic action against the amoeba. Beyond the usual predator-prey interaction terms, the model features a "Holling type" feedback term that complicates the matter.
- The growth of a tumor cell, modeled by differential equations involving random (convex) sets. Given pictures of the cell at different moments in time, we seek to recover model parameters for its growth equation. The convexity assumption means we can consider growth rates in individual directions to determine the dynamics of the frontier of the cell. The resulting infinite dimensional problem is approximated by a sequence of finite-dimensional problems.

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A Multiple Prior Monte Carlo Method for the Backward Heat Diffusion Problem

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We consider the nonlinear inverse problem of reconstructing the heat conductivity of a cooling fin, modeled by a 2-dimensional steady-state equation with Robin boundary conditions. The Metropolis Hastings Markov Chain Monte Carlo algorithm is studied and implemented, as well as the notion of priors. By analyzing the results using certain trial conductivities, we formulate several distinct priors to aid in obtaining the solution. These priors are associated with different identifiable parts of the reconstruction, such as areas with vanishing, constant, or varying slopes. Although more research is required for some non-constant conductivities, we believe that using several priors simultaneously could help in solving the problem.

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Analysis of Monotonic Discretizations for ODE Parameter Estimation

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Consider a system of ordinary differential equations (ODEs)

$$x' = f(t,x,\lambda), \qquad x \in R^m, \quad \lambda \in R^q,$$

that models some physical or biological process, and the problem of determining appropriate model parameter values λ from time series data of the model variables $\{(t^n_{\text{obs}}, x^n_{\text{obs}})\}_{n=1}^N$. Standard estimation procedures produce a point estimate λ^* which hopefully minimizes some measure of the error between the data and the model solution. These procedures are typically computationally intensive depending on the complexity of the ODE, and may converge to a local minimizer of the error measure depending on the initial estimate for λ.

As an alternative to the above procedure, consider a parameter range reduction scheme [1] where each of the q parameters is given an initial range, which at worst is the whole real line but in general is as small an interval as *a priori* information permits. The product of these ranges is a q-dimensional box in parameter space. The scheme reduces these ranges by chopping off slices of this box when it determines that the parameter values in that slice are inconsistent with the recorded data. The output of the scheme is a box or set of boxes enclosing the parameter sets that are not inconsistent with the data. Even if the volume of this output set is too large to meet the precision of the parameter identification desired by the user, it can be used to identify appropriate regions of parameter space from which to select initial parameter values to start a best point estimate algorithm of the type discussed above. Typically, this parameter range reduction scheme rapidly reduces the size of the initial parameter box and results in a much smaller space through which to search for an optimal point estimate.

The parameter range reduction scheme utilizes certain monotonic discretizations of the differential equations. Various classes of monotonic discretizations are described and their effectiveness in the range reduction algorithm is determined both analytically on a proto-type simple vector field, and empirically on more complex vector fields. It turns out that a particular class of discretizations produces the smallest ranges on the simple vector field and the reason for this is characterized. The effectiveness of each discretization class is considered in terms of the number of steps in the discretization, its order, the time step size, and the amount of noise in the data.

These discretizations can also be accumulated — the repeated process of shifting the discretization forward by one time step and adding. Accumulations allow larger time windows for the discretization function and hence incorporate more global information from the data. It is shown that if the base discretization has certain properties then accumulations of the discretization tend to have improved parameter estimation capabilities.

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Queueing Theory and Applications

SS-AQT

Organizers:
Douglas Woolford, *Wilfrid Laurier University (Canada)*
David Stanford, *University of Western Ontario (Canada)*

The talks in this session will highlight the broad scope of queueing research, providing both a mix of theory and applications. Scheduling and other aspects of congestion will be discussed in the context of traffic lights, ambulance offload delays, and transplant queues. In addition, insight into a renewal problem will be presented.

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Level Crossing Analysis of a Renewal Problem

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This talk reviews a simple renewal problem with interarrival times uniformly distributed on (0,1). The objective is to determine the expected number of renewals required to first exceed the barrier 1. The (well known) solution is obtained by using a standard renewal equation. Next the simple renewal problem is placed in a new framework, and we employ a technique based on level crossing theory (LC) to obtain the solution. Then we consider a generalization of the simple renewal problem with a barrier at a positive integer $K = 2, 3, \ldots$. The solution of the generalized problem would be complicated when using a method based on a standard renewal equation. However, by applying the technique based on LC, it is shown how to derive an explicit analytical formula for the expected number of renewals required to exceed the barrier K, in a routine manner. We also obtain an asymptotic formula for the expected number of renewals required to exceed the barrier K when K is large.

The LC method of analysis of the renewal problem can be applied directly to determine the expected number of demands during an ordering cycle of an <s,S> inventory system having no product decay, and related quantities in queues and other stochastic models.

The solution method based on LC is intuitive and may lead to new insights and generalizations.

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Two Unordered Queues

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A special customer must receive service from two independent queues with the same service rates and arrival rates. The customer can observe the current numbers at each queue prior to joining. Though it is intuitively clear that it is better to join the shorter queue first, we present an example to illustrate that this is not always the case and attempt to quantify conditions when it is better to join the longer queue. The two queues will each be M/M/1. We will use known transient M/M/1 queueing results to obtain expressions for total system time under both choices of which queue to join first.

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Delays at signalised intersections with exhaustive traffic control

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We study a traffic intersection with vehicle-actuated traffic signal control. Traffic lights stay green until all lanes within a group are emptied. Assuming general renewal arrival processes, we derive exact limiting distributions of the delays under Heavy Traffic (HT) conditions, using theory on polling models. Furthermore, we derive the Light Traffic (LT) limit of the mean delays for intersections with Poisson arrivals, and develop a heuristic adaptation of this limit to capture the LT behaviour for other interarrival-time distributions. We combine the LT and HT results to develop closed-form approximations for the mean delays of vehicles in each lane. These closed-form approximations are quite accurate, very insightful and simple to implement.

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A Markovian Queueing Model For Ambulance Offload Delays

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Ambulance offload delays are a growing concern for health care providers in many countries. Offload delays occur when ambulance paramedics arriving at a hospital Emergency Department (ED) cannot transfer care of the patient immediately. The delay occurs as they must wait in the ED until a bed is available for the patient. ED beds are allocated to both ambulance and walk-in patients, and the allocation depends on the acuity of the patient. Using queueing theory, we model the interface between an Emergency Medical Services (EMS) provider in a region, and an ED that serves both ambulance and walk-in patients. We introduce a Markov chain representation for this system and solve for the steady state probability distributions of queue lengths and waiting times using Matrix Analytic Methods. Moreover, we derive a number of performance measures used to evaluate the system when resource levels are changed. Our results indicate that if preemptive priority is assigned to patients arriving by ambulance, the ambulance offload delay is not significant. On the other hand, the impact on the waiting times of walk-in patients is significant.

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A New Paradigm for Priority Patient Selection

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The central purpose of this work is to bridge the gap between two aspects of health care systems: 1) Key Performance Indicators (KPIs) for delay in access to care for patient classes, with differing levels of acuity or urgency, specify the fraction of patients needing to be seen by some key time point. 2) Patient classes present themselves for care, and consume health care resources, in a fashion that is totally independent of the KPIs. Rather, they present in a manner determined by the prevalence of the medical condition, at a rate that may vary over time. Treatment times will likewise be determined by medical need and current practice. There is no reason to expect the resulting system performance will adhere to the specified KPIs. The present work presents a new paradigm for priority assignment that enables one to fine-tune the system in order to achieve the delay targets, assuming sufficient capacity exists for at least one such arrangement.

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A Self-promoting Priority Model for Transplant Queues

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In many jurisdictions, organ allocation is done on the basis of the health status of the patient, either explicitly or implicitly. This presentation presents a Matrix-analytic priority model in which customers self-promote to the higher priority level, to take into account changes in health status over time. In the first variant, all patients arrive as "regular" customers to the queue, but as the health of a patient degrades, their status is promoted to "priority" to reflect the increased urgency of the transplant. Performance measures such as the mean and distribution of the time until transplant are obtained.

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Computational Bio-nanotechnology

SS-BNANO

Organizers:
Hin-Hark Gan, *New York University (USA)*
Gaurav Arya, *University of California San Diego (USA)*

Computational modeling based on statistical mechanics and computer simulations is playing increasingly important roles in nanotechnology. This session shares recent progress in the development and application of such theoretical tools towards the design and understanding of RNA-based nanotechnology, single molecule transitions, DNA sequencing, ordered nano-structures, molecular motors, nano-capsules, nano-transport systems, etc.

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Recovering Single-Molecule Energetics and Kinetics from Force Spectroscopy

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Understanding how biological molecules fold into complex 3D structures, bind to each other, and undergo conformational transitions is important from the point of view of designing drugs, dissecting disease mechanisms, designing sensors, and DNA sequencing. Dynamic single molecule force spectroscopy provides a powerful approach for probing the underlying energy landscape governing such molecular processes. These sophisticated experiments operate by imposing gradually increasing forces on single molecules, or their complexes, and recording their force-extension behavior until eventual rupture. An outstanding question in this field is how to recover the intrinsic energy landscape of the molecule from such force measurements. In this talk I will describe the development of new theoretical models for extracting the height and location of activation energy barriers and intrinsic transition rates from single-molecule force measurements. The models go beyond the current state-of-the-art by accounting for both the finite stiffness of the pulling device [1] and the non-linear stretching of the molecular handles [2] often used for connecting the molecule of interest to the device.

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Multiscale modeling of biomolecular machines: insights into their structure, dynamics and function

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The binding of a substrate (i.e., small molecule ligand or protein/nucleic acid) triggers large-scale protein motions that occur on millisecond (or longer) timescales. In cell, such motions are involved in several important functions including drug binding, enzyme catalysis, allosteric regulation, protein folding, ion permeation through membrane channels, macromolecular assembly, etc. To understand this molecular recognition process more fully, it is essential to determine the corresponding mechanistic pathway as well as the underlying energy landscape of the functionally important conformational changes taking place. This, in turn, will point to ways to modulate protein function and help direct pharmacological treatments of human diseases. Solving these biomedically relevant problems requires a combination of theory, simulation, and experiment, with theory and simulation providing an atomically detailed picture of both the thermodynamics and kinetics of conformational changes and experimental tests ensuring that these models reflect accurately what is actually occurring in a cell. Unfortunately simulations typically fall orders of magnitude short of biologically relevant time scales. I will present our approach to overcome the spatial and time-scale limitations in computational modeling of large macromolecular complexes[1]. In addition, I will describe applications of multiscale computational approaches ranging from topology based mathematical modeling to physical simulations at different levels of spatial and temporal 'coarse-graining' to describe the underpinnings of protein function in a few selected macromolecular machines. Our work in describing the energy landscape and dynamic reorganization of various macromolecular machines has already yielded some fundamental insights into the physical principles that govern their biological function. I have chosen three biologically important systems adenylate kinase [2], dihydrofolate reductase [3], and the hexameric helicase motor protein [4] to exemplify the mechanistic insights that can be achieved through a simulation approach.

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Combinatorial RNA Design

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Combinatorial design is an approach for developing functional RNA molecules for application areas such as nanotechnology, synthetic biology and therapeutics. This talk describes the theoretical and computational issues related to screening and design of large RNA libraries (10^{15} sequences). The challenge of computational screening is to attain sufficiently large libraries where functional molecules can be found. The objective of designing RNA libraries is to increase the probability of finding complex structures. For library screening, we employ a combination of primary, secondary and tertiary structure methods to achieve screening of large libraries, allowing experimentalists to assess and improve the performance of RNA libraries. We design structured libraries by performing optimization of nucleotide transition probability matrices. Our methods for screening and designing large RNA libraries provide a computational framework for discovering functional RNA molecules for emerging biomolecular applications.

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Nanoparticles Composed of RNA-Bolaamphiphile Complexes Suggest Potential as a Therapeutic siRNA Delivery Vehicle as Indicated by Molecular Dynamics Simulations

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In spite of the strong potential as a therapeutic, naked siRNA delivery in vivo has some biological barriers that need to be overcome. siRNAs need to remain intact in the blood stream and they have to overcome the strong negative charges that are present on the phosphate groups of the RNA backbone when crossing biological membranes. These problems can be surmounted by covering or encapsulating the siRNA with bolaamphiphiles. Bolaamphiphiles have two positively charged hydrophilic head groups connected by a hydrophobic chain and they can form stable monolayer membrane vesicles which can encapsulate water soluble anionic molecules. In addition, bolaamphiphiles have a relatively low toxicity level when compared to lipids and can persist in the blood for long time periods. This research involves the study of RNA shape-based and vesicle-based approaches for RNA-nanoparticle formation, with the ultimate goal of developing an siRNA delivery vehicle. In the shape-based approach, we utilize differently shaped siRNA scaffolds for RNA nanoparticle-bolaamphiphile complex formation. In the vesicle-based approach, siRNAs are encapsulated inside bolaamphiphile vesicles or bound to the vesicle surface. Our explicit solvent molecular dynamics (MD) simulation results show that bolaamphiphiles rapidly cover RNA duplexes due to the strong interaction between the cationic head groups in bolaamphiphiles and the negative charges on the phosphate groups of the RNA backbone. The bolaamphiphile head groups populate both the minor and major grooves and once bolaamphiphiles associate with the RNA, the base G forms stable hydrogen bonds with the head groups of the bolaamphiphiles. It is also found that the bolaamphiphiles can associate with the RNA via strong hydrophobic interactions. Therefore, our research suggests that siRNA nanoparticle-bolaamphiphile complexes behave in a way to be a strong candidate for the development of therapeutic siRNA nanoparticle delivery vehicles.

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Coarse-grained modeling of the RNA nanostructures

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Recently, RNA has attracted much attention in bionanotechnology, where the concept of "RNA architectonics" has been proposed – a set of recipes for (self-)assembly of the RNA nanostructures of the arbitrary size and shape [1]. Small RNA building blocks were manipulated either experimentally [1] or via computer simulation [2] into the desired 2D or 3D nanostructures (squares, hexagons, cubes, tetrahedrons etc.) that can be further assembled into periodic/quasiperiodic RNA lattices.

For these large RNA aggregates, the all-atom Molecular Dynamics (MD) calculations, even if intensively parallelized, are not able to exceed the time scales of a few (tens) nanoseconds, which is by many orders of magnitude less than the duration of the slowest processes in such macromolecules (micro- to milli- to seconds). For example, we analyzed via all atom MD [3] a simple RNA nanostructure of about 13 nm in size (330 nucleotides), a hexagon-shaped "RNA nanoring". Even using the state-of-the-art computers, the realistic (fully solvated) simulation of such structure requires ~ 40 hours per nanosecond. That is why the development of a coarse grained description of RNA, suitable for simulation of large (thousands nucleotides) structures at the timescale of at least microseconds is of great importance.

In a recent study [4] we presented the initial variant of the CG model for RNA, that enabled us to perform microseconds-long Coarse-Grained MD (CGMD) simulations of the RNA nanoring with the structural precision of 0.06 Åof RMSD per nucleotide. The current version of our model includes 3 beads per nucleotide with bonded as well as non-bonded interactions between them, and it uses the idea of so-called "RNA conformation classes", which exploits the robustness of the reduced representation of the nucleic backbone in terms of backbone pseudo-dihedrals [5]. This opens up the road towards the development of a universal and highly transferable RNA CG models.

In the present study we extend our coarse-grained RNA model to describe other RNA nanostructures – "RNA tectosquares" bearing the right-angle motifs, as well as "RNA nanotube" composed of stacked RNA nanorings. Such model extension requires incorporation of the new conformation classes found in the fore-mentioned nanostructures, as well as an improved scheme for treatment of the base-pairing and stacking interaction terms.

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Differential and Integral Symbolic-Numeric Algorithms

SS-CA

Organizer:
Ekaterina Shemyakova, *University of Western Ontario (Canada)*

Hybrid symbolic-numeric algorithms in the polynomial and linear algebra setting have recently received much attention, developing a body of effective theory and a broad range of applications. This session investigates what steps can be made in symbolic-numeric algorithms for differential and integral operators. We wish to bring this subject to the attention of the computer algebra community. It is recognized that some first steps have already been made in this direction and there remain many questions to answer.

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Application of row-reduction of operator matrices to the computation of pi-flat outputs in control theory

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In applied control theory, differential flatness is an important tool for the analysis of linear differential systems. Recently, the concept has been extended to pi-flatness of time-varying systems with delay. We give a new characterisation of pi-flatness and devise an algorithm to check for pi-flatness that is based on row- and column-reduction of operator matrices.

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Approximation of $u_{xy} = \lambda(x,y)u$ by integrable PDEs

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Moutard equation

$$u_{xy} = \lambda(x,y)u \qquad (\mathscr{M})$$

has appeared first in Differential Geometry at the end of 19th century [2][3] and nowadays has numerous applications. For example in the theory of integrable 3-dimentional non-linear systems of PDE and in modern theory of solitons.

Given a partial solution $u = R$ of $(\mathscr{M})$ with some potential $\lambda = \lambda_0$, then for every additional partial solution $u = \phi$, there is a family of the corresponding solutions θ of $(\mathscr{M})$ with the potential $\lambda = \lambda_1$ defined by

$$\lambda_1 = R\left(\frac{1}{R}\right)_{xy},\ (R\theta)_x = -R^2\left(\frac{\phi}{R}\right)_x,\ (R\theta)_y = R^2\left(\frac{\phi}{R}\right)_y.$$

Continuing in the same fashion we obtain a sequence of transformations:

$$\mathscr{M}_0 \to \mathscr{M}_1 \to \mathscr{M}_2 \to \dots,$$

where $\mathscr{M}_i$ is the equation $(\mathscr{M})$ with the potential $\lambda = \lambda_i$.

Given $2k$ partial solutions of the initial equation $\mathscr{M}_0$, one can express the potential $\lambda = \lambda_k$ of the equation $\mathscr{M}_k$ and all its solutions. The formula are analogous to the "wronskian" formula for the case of the Darboux transformations for 2-dimentional integrable PDEs.

It has been also proved that the set of potentials obtainable from every fixed $\mathscr{M}_0$ is "locally dense" in the space of the smooth functions in the following sense. Let some potential λ_0 is defined in a neighborhood of $(0,0)$, then for every $N \in$ there exists potential λ^* s.t. all its derivatives $D_J\lambda^*$, $|J| \le N$ evaluated at $(0,0)$ equal to any arbitrarily chosen numbers P_J:

$$D_J\lambda^*\big|_{(0,0)} = P_J,$$

where $J = (x\dots xy\dots y)$, and $D_J = D_x\dots D_xD_y\dots D_y$.

In our talk we present our first results on the following problem: given an equation of the form $(\mathscr{M})$, find an approximation of its potential

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Stieltjes Integral Transforms: from approximate to exact values

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We consider Stieltjes functions which are functions having Stieltjes integral transforms. They have many applications in different fields of science. A Stieltjes function is defined to be the Stieltjes transform of a positive measure supported on the positive real line. We show that a number of functions built from the Lambert W function are Stieltjes. One of the analytical tools to find the measure appearing in a Stieltjes transform is the Stieltjes-Perron inversion formula which needs the evaluation of a definite integral. We investigate the possibility of computing the measure numerically when the integral is hard to evaluate analytically or even when it is not clear if the given function belongs to the class of Stieltjes functions. Examples with some functions associated with the Lambert W function and others are presented.

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Numerically stable sparse interpolation

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We consider the problem of interpolating an unknown sparse multivariate polynomial from approximate evaluations. Building upon recent work of Garg and Schost on interpolation over finite fields, we exhibit the first provably stable algorithm (in the sense of relative error) for this problem for polynomials over the complex numbers with floating-point coefficients. The number of evaluations required grows only quadratically with the number of non-zero terms, and depends only logarithmically on the degree. A key new technique is a randomization which makes all coefficients of the unknown polynomial distinguishable, producing what we call an epsilon-diverse polynomial. Another departure from most previous approaches is that our algorithms do not rely on root finding as a subroutine. We show how these improvements affect the practical performance with trial implementations.

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Using Approximate GCDs in Integral Transform Methods

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Integral transform methods can, in many cases, be used to convert initial value problems to problems in the algebra of rational functions. We explore the situation where the coefficients of the differential equations or the initial conditions are known only approximately. This leads directly to rational function arithmetic on approximate polynomials. We show how in this setting the use of approximate greatest common divisors can be used to improve solutions. This is an extension of work that was reported at ACA 2005.

AMMCS-2011

Connections between Statistics and Genetics

SS-CBSG

Organizers:
John Braun, *University of Western Ontario (Canada)*
Doug Woolford, *Wilfrid Laurier University (Canada)*

This session will highlight recent developments in the interplay between genetics and statistics. In two of the presentations, we will see how statistics is being adapted to handle high dimensional data which arises in genomics experiments, and in the third presentation, we will see how genetic evolution is inspiring new heuristic optimization approaches which find application in statistical classification and selection problems.

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Simultaneous Genetic Association Test on Multiple Traits

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A novel generalized quasi-likelihood scoring (GQLS) method is proposed to test the association between a genetic marker and a trait. The GQLS method accommodates the situation with samples of related subjects, and is flexible to test on both binary trait and quantitative trait. It can be also extended to solve the problem when sample is collected from multiple sub-populations. To date, methods in the area of genetic association studies have focused on the test of a single trait at a time. When a large number of markers are tested for association with multiple traits, controlling the overall type I error when testing traits independently becomes an issue. On the other hand, it is of great interest to identify common genetic factors that are associated with one or more than one traits. Based on our GQLS method, we develop a new method named quasi-likelihood scoring approach for multiple traits (QLSM). Simulation studies are used to validate the type I error and assess the power. Our methods will be applied to analyze real data on Canadian Holstein Cattle.

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A Marginal Mixture Model for Selecting Differentially Expressed Genes Across Two Types of Tissue Samples

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Bayesian hierarchical models that characterize the distributions of (transformed) gene profiles have been proven very useful and flexible in selecting differentially expressed genes across different types of tissue samples (e.g. Lo and Gottardo, 2007). However, the marginal mean and variance of these models are assumed to be the same for different gene clusters and for different tissue types. Moreover, it is not easy to determine which of the many competing Bayesian hierarchical models provides the best fit for a specific microarray data set. To address these two issues, we propose a marginal mixture model that directly models the marginal distribution of transformed gene profiles. Specifically, we approximate the marginal distributions of transformed gene profiles via a mixture of three-component multivariate Normal distributions, each component of which has the same structures of marginal mean vector and covariance matrix as those for Bayesian hierarchical models, but the values can differ. Based on the proposed model, a method is derived to select genes differentially expressed across two types of tissue samples. The derived gene selection method performs well on a real microarray data set and consistently has the best performance (based on class agreement indices) compared with several other gene selection methods on simulated microarray data sets generated from three different mixture models. This is a joint work with Steven Wang in Yrok University, and Qeiliang Qiu, Ross Lazarus in Harvard University.

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From Parallel Evolution to Variable-Selection Ensembles

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A few years ago, a colleague and I published an algorithm for variable selection under the title, "Darwinian evolution in parallel universes". However, only afterwards did I develop a clear, high-level understanding of what this algorithm was really doing: it was merely one way to build up what I now call a "variable-selection ensemble" (VSE). Once such a notion was formalized, it became obvious that one can build VSEs in many different ways. For example, a student and I recently built a more effective one (ST2E) by using a different generating mechanism. Some others have also emerged in recent literature. The key question, therefore, is: what makes some VSEs better than others? While an answer to this question is not yet available, I will explain in what sense we can regard ST2E's performance as being superior.

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Panel Discussion on the Connections Between Statistics and Genetics

Moderator: D.G. Woolford[1]

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A "roundtable discussion" on the connections between statistics and genetics with the presenters of the session acting as panelists.

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Minisymposium: Computational Chemistry

SS-CC

Organizers:
Ian Hamilton, *Wilfrid Laurier University (Canada)*
Randall Dumont, *McMaster University (Canada)*

Computational Chemistry uses numerical methods and algorithms to calculate properties of chemical systems which complements that obtained from experiments and which provides insight into chemical processes.

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Numerical Solution of the Dirac Equation and Applications in Laser-Matter Interaction

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This presentation will be devoted to the numerical solution of the static and time-dependent Dirac wave equation. This equation is the relativistic analogue of the Schroedinger equation and describes the dynamics of spin-$\frac{1}{2}$ particles like the electron. Its numerical solution is known to be a daunting task due to the presence of negative energy levels and the appearance of spurious fermionic states when discretizing. To solve these issues, new numerical techniques have recently been developed for the static [1] and dynamic cases [2]. The first one is a modified variational method combined with B-spline basis functions that allows to compute the bound states of a confining potential. The second one is based on the method of characteristics used in conjunction with a split operator scheme. After the description of these two techniques and a few words on their implementation, we will present results obtained for different physical systems. As a first test of the time-dependent solver, we will consider the free propagation of Gaussian wave packets, for which an analytical solution is known in 1D and 2D. On the other hand, the static solver will be validated by comparing with existing results for the ground state of diatomic molecules. Then, the time-resolved Klein paradox will be investigated. Finally, the combination of these two methods for the description of laser-matter interaction will be discussed.

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Density Functional Theory calculations on hydrated DMA-iron oxide clusters

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Methylated arsenicals include dimethylarsinic acid (DMA), which is produced in biomethylation processes of inorganic arsenic. Historically it has been used as a herbicide, and is detected in the leachates of landfills rich in waste containing arsenic such as glass, alloys, and semiconductors and biologically pretreated municipal solid waste. DMA is also synthesized during the pyrolysis of oil shale. Under certain soil solution conditions, there is potential cycling of DMA to more toxic forms of arsenic as a result of redox activity. Additionally, arsenicals (including DMA) in fossil fuels and biomass grown in As-rich soils are potent catalyst poisons hindering the optimum use and conversion of these fuels. Little is known about the surface chemistry of DMA on materials relevant to environmental systems and petroleum industry. In this talk, we present Density Functional Theory (DFT) calculations of energies, optimal geometries and vibrational frequencies for hydrated DMA-iron oxide clusters. In addition, various ligand exchange reactions are constructed for the formation of inner- and outer-sphere complexes. The Gibbs free energies of adsorption (Gads) are calculated to gain further insight into the thermodynamic favorability of adsorption. The calculations were performed on Gaussian 09, running on Sharcnet, using the B3LYP functional and the 6-31G(d) and 6-311+G(d,p) basis sets. Solvation was simulated both explicitly, by adding water molecules, and implicitly using the IEFPCM solvation model. These studies aid in the interpretation of infrared spectroscopic work in our lab on these systems, and provide geometrical parameters useful for modeling x-ray absorption data using EXAFS.

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Fitting the Electrostatic Potential for Quantum Mechanical/Molecular Mechanical Methods

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For Quantum Mechanical/Molecular Mechanical (QM/MM) methods the most problematic portion is the boundary between the MM and QM region. MM charges closest to the QM region must be pruned back to accommodate connections at the boundary, where pseudobonds or link atoms are used to connect the two regions. This often results in important electrostatic contributions being removed. Methods have been proposed such electrostatic embedding and a redistribution of the points closest to the QM region. However these methods do not fully correct the problem. Instead of modifying points at atom centers, a new method is proposed to setup a series of equally spaced out point charges on shells around the QM region, based on multiples of the Van der Waals surface. The electrostatic potential at points within the QM region is then fit using the charges on the surface formed by the shells. We show that various properties of the QM region such as charge polarization, geometries, and proton transfer barriers are correctly reproduced with our approach when compared against the ONIOM method.

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Aptamer to Ribozyme: Theoretical and Experimental Strategies for the Study of RNA based Catalysis

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The emergence of catalytic activity in RNA molecules was a crucial turning point in a hypothetical pre-RNA world. Given the relative complexity of the ribozymes that occur in nature today or have been identified by in vitro selection techniques, it is hard to envision how these molecules might have evolved from non-catalytic RNA. Studies in our group have shown that a small RNA aptamer that was .selected for its ligand binding properties possesses some intrinsic catalytic potential that allows it to accelerate an ester hydrolysis reaction. This effect is predominantly due to electrostatic transition state stabilization and was achieved without any changes to the RNA sequence or structure. Further studies have shown that the catalytic potential of this RNA is not limited to ester hydrolysis but can also be extended to other chemical reactions. We are studying the catalytic capabilities of this minimal ribozyme by a combination of theoretical and experimental approaches. Ab initio calculations are utilized to characterize the redistribution of partial charges in the substrate molecules in their bound and free conformation. The calculations are performed at various levels of theory in order to establish the optimal strategy for predicting new candidates for experimental studies of the catalytic potential of the ribozyme.

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A Computational Approach to Linear Conjugacy of Chemical Reaction Networks

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Under appropriate assumptions, the evolution of chemical reaction networks is governed by a system of autonomous polynomial differential equations over continuous variables representing the concentrations of the reactants. The resulting mass-action systems are capable of exhibiting a wide variety of qualitative behaviours, including global stability of a unique equilibrium concentration, multistability, periodic behaviour, and chaotic behaviour [1]. In [3], the authors introduce conditions under which two mass-action systems are shown to exhibit the same qualitative dynamics. This is a particularly useful approach when one of the systems has well-known dynamics while the other does not. The approach has been applied to expand the scope of complex balanced chemical reaction network theory introduced in [2].

This theory is deficient, however, in that the network with known dynamics is typically not known a priori; instead, it must be found. Even when limiting the search space to networks satisfying very restrictive conditions, such as being weakly reversible, this is typically too challenging to do by hand and must be carried out computationally. This problem has been investigated for the case of systems exhibiting the same exact system of differential equations, which are called two realizations of the given dynamics [4,5]. The authors give mixed integer linear programming (MILP) algorithms capable of finding sparse and dense realizations, as well as realizations with complex balanced equilibrium values. In this presentation, we give preliminary results which extend this approach to make use of the results contained in [3]. Importantly, these results do not require that the governing dynamical systems coincide in order to guarantee dynamical conjugacy. Our computational approach requires the efficient implementation of a mixed integer non-linear programming (MINLP) algorithm.

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Two-electron confined quantum systems: A configuration interaction approach with single-particle products and explicitly correlated wave functions

Ilya G. Ryabinkin and Viktor N. Staroverov

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Confined quantum systems of a few particles draw considerable attention as models of nanometer-sized semiconductor structures. One of the simplest confined systems is a hard-walled box containing two electrons. The electronic structure of this system is determined by the stationary Schrödinger equation with a Coulomb repulsion term, whereas the boundary conditions are determined by the shape of the box. We propose a configuration interaction (CI) method that is suitable for confining potentials with cylindrical symmetry (e.g., a sphere, a plain cylinder, a bulged cylinder, a pill-shaped box, etc.) Using our approach we explore the effect of the box shape on electron density distribution inside the box and on the formation of localized electron clumps (Wigner molecules) [1][2].

The difficulty of describing electron correlation in two-dimensional confined quantum systems is usually even greater than in 3D. In two dimensions, a configuration interaction expansion in terms of single-particle products converges so slowly as to make the method almost impractical. One way to tackle the problem is to introduce the interelectron distance into the CI wave function explicitly. We propose a special form of explicitly correlated CI that is suitable for square and rectangular boxes. We show that if the relative and center-of-mass coordinates of the two electrons are used to construct basis functions, then only basis functions that are linear in r_{12} need to be included. Using our explicitly correlated method we calculate highly accurate total energy estimates (up to 16 decimal places) for a series of squares with side lengths $L = 1, 2, 5, 10, 20,$ and 50 bohrs [3]. This accuracy is vastly superior to the mere 3–4 decimals that can be obtained at the same cost using the conventional product-based CI expansion.

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Computational Studies of Tp_2M Complexes and Their Titanium Derivatives (M = 3d transition metal, Tp^- = hydrotris(pyrazol-1-yl)borate)

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Homoleptic bis-complexes of tris(pyrazolyl)borate, $[Tp_2M]^z$, constitute the broadest constant composition motif in metal chemistry, with M spanning Ti through Zn for the 3d metals, as well as assorted heavier d-block, f-block, group 2, and p-block elements. The comparative properties of these complexes therefore provide a textbook illustration of the interplay of periodic trends, electron count, and orbital occupancy effects. We describe density functional calculations of the 3d $[Tp_2M]^{0,+}$ series and compare computed geometries and ionization potentials against experimental data. The calculations are extended further to the analysis of reaction mechanisms, activation barriers, and thermodynamics in the chemistry of Tp_2Ti (Fig. 1), the most recently discovered and most reactive member of this set (Ref. [1]). Our results calibrate the reliability of simple DFT approaches across the entire 3d series, with varying electron counts and spin states, and demonstrate the application of DFT methods to elucidate low energy barrier reaction paths in experimental synthetic chemistry.

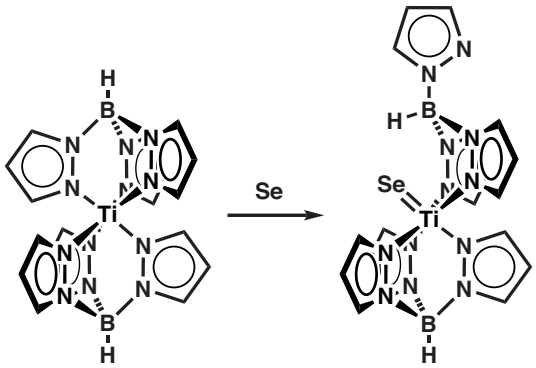

Figure 1: The reaction of Tp_2Ti with elemental selenium.

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Mixed Clusters of H_2 and H_2O: Insights from Theory and Simulations

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Water-hydrogen clusters are of considerable interest for both fundamental and practical reasons; in particular, a better understanding of their nature has implications in astrophysics and in the field of hydrogen storage. The present research investigates the quantum dynamics of water-hydrogen clusters based on a new interaction potential, exact bound-state calculations, and Feynman Path Integral simulations. We first discuss the development of a reduced-dimension effective potential for the water-hydrogen interaction. The quality of this potential is assessed by comparing the results of exact dimer and trimer bound-state calculations performed using the full-dimension and reduced-dimension surfaces both with each other and with experimental rovibrational spectra. We then perform Path Integral Monte Carlo and Path Integral Molecular Dynamics simulation of larger clusters using this newly developed effective potential, focusing on the quantum delocalization effects of *para*-hydrogen and its superfluidity in the presence of water as the size of the hydrogen clusters grow. Spectroscopic observables will be computed and compared to available experiments. This work is a prelude to an exploration of the possible impact of these quantum effects on the behaviour of nano-scale water clathrates.

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Accurate total energies from the model potential of van Leeuwen and Baerends

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In density-functional theory, there are two important ingredients that need to be treated approximately: the exchange-correlation functional and the associated potential. The latter is defined as the functional derivative of the former. In the conventional treatment, one starts by approximating the functional and then derives the potential by functional differentiation. Alternatively, one can model the potential directly and assign an energy to it as a line integral along a path of suitably chosen densities [1][2],

$$E_{\rm xc}[\rho] = \int_0^1 dt \int v_{\rm xc}([\rho_t];\mathbf{r}) \frac{\partial \rho_t(\mathbf{r})}{\partial t}\, d\mathbf{r}.$$

In 1994, van Leeuwen and Baerends proposed an approximate exchange-correlation potential, called LB94 [3],

$$v_{\rm xc}^{\rm LB94} = -\left(\frac{3}{\pi}\right)^{1/3} \rho^{1/3} - \frac{\beta \xi \rho^{1/3} s^2}{1 + 3\beta\xi s \sinh^{-1}(\xi s)},$$

where $s = |\nabla\rho|/\rho^{4/3}$, $\xi = 2^{1/3}$, and $\beta = 0.05$ is an empirical parameter. The LB94 potential yields excellent ionization energies due to the improved asymptotic behavior, but the total energies calculated with this approximation are in serious error. The reason for this failure is that the LB94 potential is not a functional derivative of any density functional, so the energy assigned to it depends on the integration path. In this work, we compare the energies computed using two distinct parametrizations of the density: (a) the uniform scaling $\rho_\lambda(\mathbf{r}) = \lambda^3 \rho(\lambda \mathbf{r})$ and (b) linear density scaling $\rho_q(\mathbf{r}) = q\rho(\mathbf{r})$. The parametrization (b) has not been used to assign energies to model potentials prior to our study. We found that the energies evaluated with the linearly-scaled density (b) are significantly lower than the exact energies, and traced the origin of this problem to the empirical parameter β. Using a revised value of β we constructed a new accurate generalized-gradient approximation whose functional derivative is closely related to the LB94 potential.

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Non-local Uniform Electron Gas based Functionals for Real Systems

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Due to its favourable cost per unit accuracy, density functional theory (DFT) is recognized as the method of choice for computing the electronic structure of large molecules and complex materials. In it the exchange-correlation functional has to be approximated since its exact form is unknown. Several models have been proposed for it. Some of them, such as PBE and TPSS, are exact for the uniform electron gas, an important constraint in DFT. In this contribution we compute the exchange-correlation energy based directly on the hole for the uniform electron gas. This functional provides a non-local "two-point" model for the exchange-correlation hole instead of a one for the exchange-correlation energy density. Normalization on the hole is enforced in order to analyze the impact of this constraint in the proposed model. Results are presented before and after normalization and compared to the aforementioned functionals.

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Addressing the Coulomb Potential Singularity: A Basis Set Approach

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When performing calculations in density functional theory (DFT) the energy is given by the sum of several contributions. Particularly the electron repulsion and the exchange-correlation energy (when expressed in terms of the exchange-correlation hole) integrals present a difficulty. When two electrons are very close one to another the value of the Coulomb potential tends to infinity. Numerical tools in order to tackle this difficulty are of general interest when performing Quantum Chemistry calculations. In this contribution we present a tool to address this difficulty. This one is based on the construction of density- and potential- like basis sets that allow managing the Coulomb singularity in a formal and analytical fashion. Some results for simple systems are presented.

AMMCS-2011

Minisymposium: Complex Dynamics of Population Behaviour with Impact to Socio-Economic Issues

SS-CDPB

Organizers:
Monica Cojocaru, *University of Guelph (Canada)*
Christopher Hogg, *University of Guelph (Canada)*
Veronica Gheorghiade, *University of Guelph (Canada)*

This minisymposium is aiming to bring together talks on topics related to population behaviour and socio-economic issues using different modelling paradigms. The investigations to be presented rely on dynamic models of behaviour encompassing continuous and discrete dynamics. In most cases, the underlying applications drive the modelling and computational approaches, ranging from cellular automata and agent-based models to ordinary and partial differential equations.

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Additive representation of separable preferences over infinite Cartesian products

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Let $\mathscr{X}$ be a set of states, and let $\mathscr{I}$ be an infinite indexing set. For example, $\mathscr{I}$ could represent a sequence of moments in time, a set of possible 'states of nature', or a set of persons. Meanwhile, $\mathscr{X}$ could be a set of material goods, or the set of psychophysical states available to an individual. An element $\mathbf{x}$ in $\mathscr{X}^{\mathscr{I}}$ represents an assignment of a state x_i in $\mathscr{X}$ to each element i of $\mathscr{I}$. Many problems of either individual or collective decision-making require us to impose a *preference order* (a complete, transitive, binary relation) on $\mathscr{X}^{\mathscr{I}}$.

Roughly speaking, a preference order $(\succeq)$ is *separable* if it is possible to hold the values of some $\mathscr{I}$-coordinates constant, and thereby obtain a consistent preference order over all possible values of the remaining coordinates. The preference order $(\succeq)$ is *permutation-invariant* if $\mathbf{x} \approx \mathbf{y}$ whenever $\mathbf{y}$ is obtained by permuting any finite number of coordinates in $\mathbf{x}$. For example, if $\mathscr{I}$ represents a sequence of moments in time, then permutation-invariance means that $(\succeq)$ exhibits no 'impatience' or other time-preferences. If $\mathscr{I}$ represents a set of persons, then permutation-invariance means that $(\succeq)$ is impartial.

We show that any separable, permutation-invariant preference order $(\succeq)$ on $\mathscr{X}^{\mathscr{I}}$ admits an additive representation. That is: there exists a linearly ordered abelian group $\mathscr{R}$ and a 'utility function' $u : \mathscr{X} \longrightarrow \mathscr{R}$ such that, for any $\mathbf{x}, \mathbf{y} \in \mathscr{X}^{\mathscr{I}}$ which differ in only finitely many coordinates, we have $\mathbf{x} \succeq \mathbf{y}$ if and only if $\sum_{i \in \mathscr{I}} [u(x_i) - u(y_i)] \geq 0$. In most 'utility representation' theorems in theoretical economics, $\mathscr{R}$ is assumed to be the additive group $\mathbf{R}$ of real numbers. However, in our framework, $\mathscr{R}$ could also be the additive group $\mathbf{R}^n$ with the lexicographical order, or the additive group ${}^*\mathbf{R}$ of hyperreal numbers. Thus allows $(\succeq)$ to represent 'non-Archimedean' preferences, where some goods or values are given infinite priority over other goods or values.

If $(\succeq)$ also satisfies a weak continuity condition, then, for *any* $\mathbf{x}, \mathbf{y} \in \mathscr{X}^{\mathscr{I}}$, we have $\mathbf{x} \succeq \mathbf{y}$ if and only if ${}^*\sum_{i \in \mathscr{I}} u(x_i) \geq {}^*\sum_{i \in \mathscr{I}} u(y_i)$. Here, ${}^*\sum_{i \in \mathscr{I}} u(x_i)$ represents a 'hypersum': an infinite summation operator defined using methods from non-standard analysis. The hypersum takes values in a linearly ordered abelian group ${}^*\mathscr{R}$, which is an ultrapower extension of $\mathscr{R}$. Like an integration operator or series summation operator, the hypersum allows us to define the sum of an infinite set of values. However, unlike these operations, the hypersum does not depend on some form of convergence (recall: $\mathscr{R}$ has no topology) —it is always well-defined. Also, unlike an integral, the hypersum does not depend upon a sigma-algebra or measure on the indexing set $\mathscr{I}$.

These results are applicable to infinite-horizon intertemporal choice, choice under uncertainty, and variable-population social choice.

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An agent-based model of stock market investors with social network effects

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This work extends an existing cellular automata model of market investors' interaction when they are considered socially connected and the effect their behaviour has on the prices of market instruments. We take here an agent-based approach to their interactions, which helps us investigate further properties of the effects of social connectivity on their decision making (buying, selling or holding). In particular, we consider them related over three types of social networks; we further assume that each agent is influenced in a different manner by various others, and that an agent's social links can evolve (appear or disappear), making the underlying network structure time dependent.

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Significance and Complexity of the Impacts of Land Market on Land Use Change: An Agent-based Experiment

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Land use change in a market economy, particularly at the urban-rural fringe in North America, is shaped by land markets, which in turn influence land management. Although land market activities are at the core of economic studies of land use change and urban economics, many elements of land market are neglected by coupled human-environment models. Further, even econometric models of land-use change fail to represent land market elements.

In our current work, the effects of three key market elements—utility maximization, budget constraints, and competitive bidding—on outcomes in land-use change models are scrutinized through an abstract agent-based model. We explore the magnitude of the impacts of these market elements under different landscape and agent settings. In particular, our experiments investigate the extent to which resource constraints and competitive bidding shift land development and land rent patterns and alter the quantity of change projected by a land-use model, holding everything else equal. We calculate two groups of measures, spatial and economic, to delineate the variation of simulated landscapes under different market levels.

Our results show that while incorporating market components in land use models, in general, alters projected land use patterns, their impacts are significantly different under various conditions. Consistent with land change theories and existing evidence, the model reconfirms that resource constraints can considerably reduce the projected quantity of land use changes. Unlike resource constraints, the effect of competitive bidding is more complex, primarily because of interactions with agent heterogeneity in preferences, budget levels, and perception of neighborhood quality. With our specific model settings, competitive bidding may not always increase average transaction price and total social welfare. Moreover, while competition induces more compact land development patterns under certain conditions, it may also encourage sprawled patterns through market sorting. Explicitly representing land market elements, therefore, is necessary to accurately project land changes and to characterize the complexity inherent in coupled human-environment systems.

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Social Interaction Dynamics and Their Effect on New Product Adoption

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In this talk, we present a partial differential equation model to describe the social interactions and evolution of preferences by consumers within a population. We encorporate a differentiated product market setting in which we look to describe the eco-product as a variant of a product already on the market. Through a previously developed extension of the characteristics model to a time dependent one, we develop a system of convection-diffusion equations to model two types of consumers, Innovators and Imitators, within our population. Innovators are those who purchase the product with no previous knowledge of it, and Imitators are those who purchase the new product based on the opinions of others. We extend the model to higher dimensions to include both horizontal and vertical product differentiation. We present numerical simulations of the model as well as present an application to a real world example using data collected from a recent survey. In closing, we discuss our findings and the direction of future work from this research.

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The network of sponsored search auctions

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Most Web search engines like Google, Yahoo! and Bing auction space next to their generic search results, a practice known as sponsored search auction (also known as *keyword auction*). Sponsored search is now an indispensable part of the business model of modern web hosts. Currently, the overwhelming majority of the search engines' revenue comes from sponsored search: In 2009, Google's sponsored search generated $22 billion that is 97% of its revenue.

In a typical model of sponsored search auctions, advertisers participate in a General Second Price Auction and bid for placement on available slots on the page where the advertiser with a higher bid is more likely to appear above other advertisements on the page (See [3]. So advertisers are competing with providers of the same products and/or services. Indeed, it is widely believed that advertisers impose externalities on each other; the value of a slot depends on the identity (and position) of the other advertisers (See [1]).

We study the large-scale network of the sponsored search advertisers on Google (See [2]), Yahoo! and Bing. To model these networks, two advertisers are connected if they compete for the same keyword (of a set of almost one million keywords). We show that in all three cases, the network is small-world and scale-free. In fact, the network has the same properties when only a particular category of keywords are considered. However, to our surprise, some of the fundamental parameters of these three networks are different.

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Shopkeeper Strategies in Iterated Prisoner's Dilemma

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A large number of studies have evolved agents to play the iterated prisoner's dilemma. This study models a different situation, called the Shopkeeper model of interaction, in which a state conditioned agent interacts with a series of other agents without resetting its internal state. This is intended to simulate the situation in which a shopkeeper interacts with a series of customers. In a majority of other studies agents either reset their internal state information before each new encounter or have relatively little internal state information. This means they cannot model situations such as being the customer after the customer from hell. We train shopkeeper prisonerâs dilemma agents against a variety of distributions of possible customers. The shopkeepers specialize their behavior to their customers but sometimes fail to discover maximally exploitative behaviors. The evolved shopkeeper agents are subject to fingerprint analysis and are shown to differ substantially from agents evolved with a round-robin fitness functions. Evaluation of the behavior of the shopkeeper agents with customers they did not encounter during evolution provides additional evidence that shopkeepers specialized to the customers, but did so incompletely for the more complex sets of customers.

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A Linear Programming Network Analysis of Phosphorus Reduction Strategies for the Lake Simcoe Watershed

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To promote the health of the Lake Simcoe watershed, the Lake Simcoe Phosphorus Reduction Strategy (2010) has adopted an explicit goal of reducing annual phosphorus loadings from the current average of 72T/yr to a target of 44T/yr. Unfortunately, phosphorus is the product of numerous and varied human processes, spread amongst a heterogeneous group of individuals and institutions who have differing capacities for lowering emissions. Achieving this target therefore, represents an enormous challenge for government agencies who must not only identify/project phosphorus emissions but must also control/influence emitters. Our approach aims to provide decision support tools to assess and support strategic phosphorus reduction strategies within the Lake Simcoe Watershed.

Our framework utilises a suite of complementary methodologies to examine the assumptions of the proposed phosphorus reduction frameworks and their targets, as well as hybrid approaches suggested by modeling results. For the first stage of mathematical analysis we have constructed WetNet V1.0 as a linear programming network model that is capable of sifting through numerous decision possibilities to provide a feasible/efficient regulatory prescription. The model's task is to schedule a sequence of regulatory measures among and between various actors, to meet overall phosphorus load constraints. This well-established, top-down approach is simple, transparent and captures efficiencies that would be missed in a disaggregated cost/benefit analysis. It also allows for a feasibility assessment of system targets given reasonable expectations regarding technological improvements, dynamic time preferences, and the economic viability of various investments.

In the second stage of development we will be generating a simulation model as a complement to WetNet's strategic analysis. This bottom-up, agent based modeling (ABM) approach allows us to more precisely model emitters and regulators (i.e. individual actors), the costs and benefits associated with phosphorus emission (i.e. their currencies), technology options (i.e. their strategy sets) and regulation (i.e. the constraints imposed upon them). It will also allow representation of the interactions between individual emitters and regulators (i.e. actors within various populations over time). The result is a more precise representation of individual phosphorus emission activities and agent response to incentive/disincentives, within a spatially explicit, and ecologically appropriate environment.

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New product adoption with dynamic consumer preferences and endogenous pricing

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We examine a pricing game between firms that produce differentiated products and in which consumer preferences evolve in response to the market shares of the available products. One of the products is new and a subset of consumers (early adopters) have a relatively strong preference for it, while the remaining consumers are influenced by the relative market shares of the two products, being drawn to the product with the higher market share. We use a system of PDEs to specify the evolution of the preferences for the alternative goods. This system is nonlinear due to the influence of existing consumption choice on the distribution of preferences. The pricing game allows firms to react to the changing distribution of consumer preference. We find that allowing for the evolution of consumer preference in this way results in interesting dynamics for prices. In particular, price paths can be non-monotonic over time.

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Minisymposium: Computational Methods for Hyperbolic Problems

SS-CMHP

Organizers:
Jae-Hun Jung, *SUNY at Buffalo (USA)*
Allen Tesdall, *CUNY College of Staten Island (USA)*

Hyperbolic conservation laws describe a wide range of wave propagation and fluid flow phenomena, including shock waves in nonlinear situations. In the last several decades important advances have been made in the numerical computation of accurate solutions to these problems. In this minisymposium, recent results in the theory and application of these methods will be presented. A variety of computational techniques, including but not limited to finite volume, finite element, spectral, WENO, and discontinuous Galerkin methods, will be represented.

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Modeling and Risk Analysis of Volcanic Mass Flows

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Mass flows consequent to volcanic eruptions range from the slow efflux of lava to the rapid flow of hot pyroclastic materials to the muddy mess of debris flows. We will discuss the modeling of these mass flows, and in particular the modeling issues associated with the fluid plus solid materials debris flows. We outline a 'thin layer' approximation for two phase flows, akin to shallow water models. We discuss the strengths and limitations of such models and the prospects for more general two phase models. We also discuss the inputs to simulations of volcanic mass flows for hazard analysis - the inputs and their uncertainties, the kinds of outputs that are useful to those concerned with civil protection. We discuss the kinds of statistical analysis that are necessary to construct a true hazard map for a volcano. This work is part of a large collaborative effort, supported by various NSF awards. I am reporting on results obtained in joint efforts with Abani Patra, Eliza Calder, Mike Sheridan, Marcus Bursik, Long Le, Jim Berger, Susie Bayarri, Robert Wolpert, Keith Dalbey, and Fei Liu.

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Numerical Solution of Non-Equilibrium Gaseous Flows Using Hyperbolic Moment Closures

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The numerical solution of the first-order hyperbolic systems of weak conservation equations that result from maximum-entropy moment closures for the Boltzmann equation of gas-kinetic theory is considered. The maximum-entropy closures provide hyperbolic transport equations for an extended set of fluid-dynamic properties that, unlike conventional continuum descriptions, can account for the evolution of gases both in and significantly far from local thermodynamic equilibrium. The use hyperbolic moment equations for numerical prediction of gaseous flows can also present several numerical advantages. A parallel, implicit, adaptive mesh refinement (AMR), upwind, finite-volume scheme is described for the solution of the 10-moment equations of the Gaussian closure and applied to the prediction of a range of three-dimensional, non-equilibrium, gaseous flows. The Gaussian maximum-entropy closure and provides a fully-realisable and strictly hyperbolic description of non-equilibrium gaseous flows that is valid from the near-equilibrium or continuum limit, through the transition regime, up to the near free-molecular flow limit. Although this somewhat simplified mathematical model does not incorporate the effects of heat transfer, it is very representative of other higher-order closures. The proposed upwind scheme makes use of Riemann-solver-based flux functions and limited linear reconstruction to provide accurate and monotonic solutions, even in the presence of large solution gradients and/or under-resolved solution content on three-dimensional, multi-block, body-fitted, hexahedral mesh. A block-based AMR strategy is adopted herein to allow for local refinement of the computational mesh. A rather effective and scalable parallel implicit time-marching scheme based on a Jacobian-free inexact Newton-Krylov-Schwarz (NKS) approach with additive Schwarz preconditioning and domain partitioning following from the multi-block AMR mesh is used for the solution of the non-linear ordinary-differential equations that result from the application of the upwind spatial discretization procedure. Numerical results for several canonical flow problems are describe to demonstrate the predictive capabilities of the approach for fully three-dimensional, non-equilibrium, gaseous flows.

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Convection-dominated problems in a circle domain

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In this article we aim to study the boundary layer generated by a convection-diffusion equation in a circle. In the model problem that we consider two characteristic points appear. To the best of our knowledge such boundary layer problems have not been studied in a systematic way yet and we indeed know that very complex situations can occur. In the cases that we consider in the present article certain simplifying compatibility conditions are assumed. Other situations will be addressed which involve noncompatible data, or more general domains.

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Conservative discontinuous Galerkin methods for the generalized Korteweg-de Vries equation

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The Korteweg-de Vries (KdV) equation is a nonlinear mathematical model for the unidirectional propagation of waves in a variety of nonlinear, dispersive media. Recently it has attracted increasing attention as test-bed for the competition between nonlinear and dispersive effects leading to a host of analytical issues such global existence and finite time blowup, etc. In this presentation, we construct, analyze, and numerically validate a class of conservative discontinuous Galerkin schemes for the generalized KdV equation. The schemes preserve the first two invariants (the integral and L2 norm) of the numerical approximations. We provide numerical evidence that this property imparts the approximations with beneficial attributes such as more faithful reproduction of the amplitude and phase of traveling wave solutions.

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A New Look at Singular Shocks

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Some examples of singular shocks, which are solutions of conservation laws of very low regularity, were found by Herbert Kranzer and the speaker in the 1980's, and a theory was developed by Michael Sever that encompassed the examples, and categorized the differences between singular shocks and delta shocks, another type of low- regularity solution. However, the topic has remained merely a curiosity until recently.

Now, some new models, numerical simulations and experiments in chromatography suggest that these somewhat pathological waves may have a physical meaning, and that the examples studied so far may not cover the entire spectrum of singular behavior of solutions of conservation laws. This talk will summarize what is known, and what might be conjectured about delta and singular shocks.

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Central discontinuous Galerkin methods for ideal MHD equations with the exactly divergence-free magnetic field

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In this talk, high order central discontinuous Galerkin methods are developed for solving ideal magnetohydrodynamic (MHD) equations. The methods are based on the original central discontinuous Galerkin methods designed for hyperbolic conservation laws on overlapping meshes, and use different discretization for magnetic induction equations. The resulting schemes carry many features of standard central discontinuous Galerkin methods such as high order accuracy and being free of exact or approximate Riemann solvers. And more importantly, the numerical magnetic field is exactly divergence-free. Such property, desired in reliable simulations of MHD equations, is achieved by first approximating the normal component of the magnetic field through discretizing induction equations on the mesh skeleton, namely, the element interfaces. And then it is followed by an element-by-element divergence-free reconstruction with the matching accuracy. Numerical examples are presented to demonstrate the high order accuracy and the robustness of the schemes.

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Efficient high-order time integration algorithms for transport simulations

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We investigate efficient algorithms and a practical implementation of an explicit-type high-order timestepping method based on Krylov approximations, for possible application to large-scale engineering problems in electromagnetics and fluids. We consider solving a semi-discrete form of the Maxwell equations for electromagnetics and a lattice Boltzmann equation for single phase flows, resulting from a high-order spectral-element discontinuous Galerkin discretization in space whose solution can be expressed analytically by a large matrix exponential of dimension *nxn*. We project the matrix exponential into a small Krylov subspace by the Arnoldi process based on the modified Gram-Schumidt algorithm and perform a matrix exponential operation with a much smaller matrix of dimension *mxm*. For computing the matrix exponential, we obtain eigenvalues of the *mxm* matrix using available library packages and compute an ordinary exponential function for the eigenvalues. The scheme involves mainly matrix-vector multiplications, and its convergence rate is generally order $(m-1)$ in time so that it allows taking a larger timestep size as *m* increases. We demonstrate CPU time reduction compared with results from the five-stage fourth-order Runge-Kutta method for a certain accuracy. We also demonstrate error behaviors for long-time simulations.

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A Discontinuous Galerkin Method for Hyperbolic Problems on Cartesian Grids with Embedded Geometries

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Methods based on Cartesian grids with embedded geometries are an alternative approach to computations performed on unstructured grids. Generation of Cartesian grids is significantly simpler than generation of unstructured meshes around complex geometries. They also provide significant computational savings on the majority of regular grid cells as the uniform size, shape, and orientation of mesh elements allows us to reduce both computing time and storage requirements. This might be especially important for computationally intensive high-order schemes such as the discontinuous Galerkin methods. However, the major challenge of the discontinuous Galerkin method on Cartesian grids is the so called cut cells that arise from cutting out a geometry from the computational domain. They are difficult to deal with due to their small size and irregular shapes. Arbitrarily small size of cut cells leads to a restrictive CFL condition imposed on the whole mesh while explicit scheme is used. Irregular shapes are difficult to integrate on due to absence of integration rules, and also need extra storage for special quadrature rules on each cut cell. We present an approach of dealing with cut cells based on merging of cut cells with neighboring elements. This alleviates the CFL restriction but resulting merged cells might have irregular shapes depending on the shapes of cut cells. We discuss how to deal with integration on such elements with the aim to preserve accuracy and without resolving to refining mesh near the embedded boundary. Since the available bounds of time step guaranteeing a stable solution are overly conservative, how to impose the CFL condition on several types of cut cells will also be discussed. Numerical results will be shown to validate the efficiency of the proposed approach.

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Some Remarks On the Numerical Approximation of One-Dimensional Non-conservative Hyperbolic Systems

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The aim of this talk is to lay a theoretical framework for developing numerical schemes for approximating one-dimensional Non-Conservative Hyperbolic Systems (NCHSs). These systems arise in a wide variety physical and industrial applications, but they are far less understood than their conservative counterparts. We first recall some key points of the theory of NCHSs, beginning with the definition of non-conservative products proposed by Dal Maso, LeFloch, and Murat (DLM) [1]. Next, we briefly introduce the vanishing viscosity solutions and shock curves derived from Bianchini and Bressan [2], and their partial generalization proposed by Alouges and Merlet [3]. Approximation of these shock curves also proposed by Alouges and Merlet are then introduced and discussed. We then investigate the numerical implementation of these analytical approaches using in particular, Godunov-like schemes, with either using the approximate Shock curves of Alouges and Merlet directly in a Riemann solver, or within the DLM-path theory framework (see [4]). The convergence of these schemes will be discussed, and illustrated by several numerical examples.

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Strong-stability-preserving 7-stage HB methods

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Optimal, 7-stage, explicit, strong-stability-preserving (SSP) Hermite–Birkhoff (HB) methods of orders 4 to 8 with nonnegative coefficients are constructed by combining linear k-step methods with a 7-stage Runge–Kutta (RK) method of order 4. Compared to Huang's hybrid methods of the same order, the new methods generally have larger effective SSP coefficients and larger maximum effective CFL numbers, num_{eff}, on Burgers'; equation, independently of the number k of steps, especially when k is small for both methods. Based on num_{eff}, some new methods of order 4 compare favorably with other methods of the same order, including RK104 of Ketcheson. The SSP property of the new HB methods are obtained from their Shu–Osher representation.

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High Order Positivity Preserving ENO and DG Methods for Hyperbolic Equations

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A class of high-order positivity preserving methods for ENO and DG methods are described. The methods are based upon a class of high-order data-bounded polynomials on general meshes will be given. Such polynomials make it possible to circumvent the problem of Runge-type oscillations on evenly spaced meshes by adaptively varying the stencil and order used, but at the cost of only enforcing C0 solution continuity at data points. It will be shown that the use of these high-order provably data-bounded polynomials, provides a way to develop positivity preserving polynomial approximations as well as methods of potentially high orders for hyperbolic equations. The central idea is to use ENO (Essentially Non Oscillatory) type approximations but to e nforce additional restrictions a class of high-order data-bounded polynomials on general meshes will be given. Such polynomials make it possible to circumvent the problem of Runge-type oscillations by adaptively varying the stencil and order used.It will be shown that the use of these high-order provably data-bounded polynomials, based on extensions of the work of provides a way to develop positivity preserving polynomial approximations as well as methods of potentially high orders for hyperbolic equations.

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Spectral methods for nearly hyperbolic problems in lake hydrodynamics

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The majority of Canada's land surface is dotted with lakes of varying size. On the Canadian Shield these lakes generally have both complex shapes and bathymetry. The hydrodynamics of these lakes is primarily driven by the wind, but during the ice free months the majority of lakes will exhibit some thermal stratification, with warmer, lighter water overlying colder, denser water. Density stratification provides a wave guide for gravity waves and the motion in the interior of lakes thus becomes a complex interplay between the generation, propagation and dissipation of waves on the surface and in the interior of lakes. The hydrodynamics influences the chemical cycles in the lake through turbulent mixing and sediment resuspension, this in turn influences lake ecology both on microscopic (plankton) and macroscopic (fish) scales.

In this talk we present spectral methods for weakly nonhdyrostatic dynamics in small and medium sized lakes. The governing equations extend the well known shallow water equations and as such are hyperbolic to leading order. We demonstrate how weak nonhydrostatic effects preclude the formation of shocks and discuss pseudospectral methods for the solution of the system of equations. Subsequently we extend Fourier-based methods to methods that use Chebyshev polynomials. These methods can account for simple closed geometries, and the example of a torus shaped lake will be discussed in detail, with a focus on the dynamics of nonlinear, coastally trapped waves. Finally, we will present spectral methods for the coupled problem of lake dynamics and the flow in a porous lake bottom. We discuss the challenges inherent in the mismatch of length scales and reynolds numbers, and will present selected numerical examples.

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Global solutions for transonic two-dimensional Riemann problems

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We discuss the recent development of transonic two-dimensional Riemann problems. We present the existence results for the global solutions to certain configurations. We also present some numerical results as well.

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Self-similar solutions for the diffraction of weak shocks

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We formulate a problem for the unsteady transonic small disturbance equations that describes the diffraction of a weak shock near a point where its strength approaches zero and the shock turns into an expansion wave. Physically, this problem corresponds to the reflection of a weak shock wave by a semi-infinite screen at normal incidence. We formulate the equations in special self-similar variables, and obtain numerical solutions using high resolution finite difference schemes. Our solutions appear to show that the shock dies out at the sonic line, a phenomenon which has not been previously observed.

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The Modified Buckley-Leverett equation

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The focus of the present study is the modified Buckley-Leverett (MBL) equation describing two-phase flow in porous media. The MBL equation differs from the classical Buckley-Leverett (BL) equation by including a balanced diffusive-dispersive combination. The dispersive term is a third order mixed derivatives term, which models the dynamic effects in the pressure difference between the two phases. The classical BL equation gives a monotone water saturation profile for any Riemann problem; on the contrast, when the dispersive parameter is large enough, the MBL equation delivers non-monotone water saturation profile for certain Riemann problems as suggested by the experimental observations. In this talk, we first show that the solution of the finite interval $[0,L]$ boundary value problem converges to that of the half-line $[0,+\infty)$ boundary value problem for the MBL equation as $L \to +\infty$. This result provides a justification for the use of the finite interval boundary value problem in numerical studies for the half line problem. Furthermore, we extend the classical central schemes for the hyperbolic conservation laws to solve the MBL equation which is of pseudo-parabolic type. Numerical results confirm the existence of non-monotone water saturation profiles consisting of constant states separated by shocks.

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A hybrid radial basis function method for numerical solutions of vascular flows

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Detailed configuration of hemodynamics in human vasculature is a crucial part for successful surgical judgment and treatment. Vascular flows in most areas of the vasculature can be described as laminar flows, but some can be turbulent near irregular geometric areas such as bifurcations, stenoses, and aneurysms. These turbulent flows can cause significant issues in healthy hemodynamics. Thus, obtaining accurate flow behaviors around these areas is an important task.

High-order numerical methods such as the spectral method and the high-order finite difference method can be used to capture such complex fluid behaviors. These methods, however, need a strict grid restriction for the complex geometry of a blood vessel. To redeem this issue, we develop a hybrid radial basis function (RBF) method. The RBF method is known as a mesh-less method and yields high-order accuracy for smooth problems. Hence, with the RBF method, a complex geometry can be easily adopted and a high-order accuracy can be obtained.

The idea of the proposed method is to hybridize the high-order method and the RBF method. For the smooth area, a high-order method such as the spectral method is implemented and high-order accuracy is obtained with a relatively small grid resolution, while the complex geometry is efficiently covered by the RBF method with high flexibility of the grid distribution. To make the hybridization function properly, we develop an efficient and stable patching algorithm between the high-order method and the RBF method. Numerical results will be presented for several different types of blood vessels including the stenotic flows.

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Causality indicators for discontinuous Galerkin fast sweeping methods

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In this talk, I will present our recent work on developing uniformly accurate DG fast sweeping methods for solving Eikonal equations. In order to achieve both high order accuracy and fast convergence rate (linear computational complexity), the central question is how to enforce the causality property of Eikonal equations in the compact DG local solver. We design novel causality indicators which guide the information flow directions for the DG local solver. The values of these indicators are initially provided by the first order finite difference fast sweeping method, and they are updated during iterations along with the solution. We observe both a uniform second order accuracy in the L^∞ norm (in smooth regions) and the fast convergence speed (linear computational complexity) in the numerical examples.

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Uncertainty quantification for the critical phenomenon of nonlinear optics equations with a point-like impurity using the generalized polynomial chaos method

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We consider the Klein-Gordon and sine-Gordon equations with a point-like impurity. The impurity is modeled by the Dirac-δ function. The kink dynamics produced by the impurity is rich mathematically such as the fractality and the critical behavior of the kink solution. In the last decade these solution behaviors have been actively investigated with the deterministic equation. As the point-like defect is defined in a highly localized region, however, several uncertainties can be involved in the model equation and the uncertainty quantification is needed.

In this work, we investigate the kink interactions with the singular impurity when uncertainties are involved. We use the generalized polynomial chaos (GPC) method to expand the solution in the random space with the orthogonal polynomials. We also investigate how the uncertainty analysis can be used to understand the point-like impurity based on the measured data. We propose a robust GPC method to find the critical value that yields the critical phenomenon of the solution. Numerical examples will be provided, which show that the proposed method is highly accurate compared to the critical value finding method based on the Monte Carlo approach.

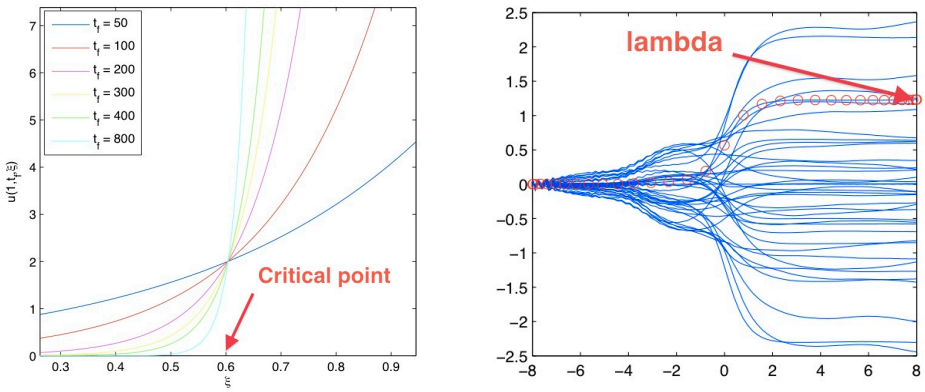

Figure 1: Finding the critical values. Left: Klein-Gordon solution with GPC method. Right: PC modes of the sine-Gordon solution with GPC method. The red circles represent the first mode $\hat{u}_0$ which is the mean of $u(x,t,\xi)$. For the sine-Gordon solution, the critical value of V_c is found by $V_c = V_a + (V_b - V_a)\lambda/2\pi$.

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Computational Nanophotonics

SS-CNP

Organizers:
Marek Wartak, *Wilfrid Laurier University (Canada)*
Brian West, *Wilfrid Laurier University (Canada)*

Recent technological advances have made possible the field of nanophotonics, the manipulation of optical fields in nanoscale dielectric and metallic environments. This area of study shows great promise in such diverse applications as medical diagnostics, optical computing, optical communications, and homeland security; however, it also introduces new challenges in device modeling. This special session is being organized to share recent developments in the computational aspect of nanophotonics.

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Nano-Scale Photonic Crystal LED Modeling by a Highly Efficient Hardware Accelerated FDTD Method

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Utilizing the photonic crystals to improve the light extraction efficiency of the light emission diode (LED) has attracted a lot of researchers' attention[1]. The optical properties of the photonic crystal LED are intensively studied with finite-difference time-domain (FDTD) method. However the FDTD method is extremely memory and time consuming[2] when dealing with the photonic crystal LED simulation problems. The main reasons are 1) the small feature size of the nano-scale structures requires very fine meshes both in spatial and time domain; 2) precisely modeling of the dispersive materials increases the computational complexity and memory requirement. Therefore it is strongly demanded to have a tool which can significantly reduce the large memory requirement and dramatically improve the simulation efficiency.

In this paper, a step wavelength scheme is proposed for studying the light extraction efficiency of the photonic crystal LED with the FDTD method. In this scheme, the lightwave of one specified wavelength is emitted by multiple noncoherent excitation sources in each simulation step. This method avoids utilizing the complex dispersion models such as multipole Drude-Lorentz model in the FDTD simulation so that the memory requirement is dramatically reduced . It also reduces the computational complexity by avoiding the Fourier transform in the computing process. By taking advantages of the inherent parallel nature of the FDTD method, the new algorithm is implemented on a graphics processing units (GPUs) cluster using the compute unified device architecture (CUDA)[3]. It is demonstrated that the high-performance computing technique leads to a significant acceleration of the FDTD simulation with more than 100 times improvement in computational efficiency in comparison with the conventional FDTD method running on CPU of a standard desktop computer.

Therefore, the new method significantly reduces the memory requirement and dramatically improves the simulation efficiency compared with traditional methods. It may serve as an efficient, accurate and robust tool for studying the light extraction efficiency of the photonic crystal LED.

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Asymmetric transition states in quantum dots

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We present a model for the shape transitions in strained solid films with strongly anisotropic surface energy. The model is formulated as a free boundary problem for the minimization of surface energy and elastic strain energy of piecewise continuous "island" shapes. In the absence of substrate miscut, it is known that a truncated pyramid minimizes the energy at small volume while a dome minimizes the energy at larger volume. Here we demonstrate the existence of an asymmetric "half-dome" shape which acts as a low-barrier metastable transition state in the transition from the truncated pyramid to dome. Thus, in a system with moderate fluctuations, half-dome quantum dots should be observed, if only rarely. We also determine that in the presence of a miscut substrate, "half-pyramid" and "half-dome" shapes can be stable equilibrium states.

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Unconditionally Stable Numerical Method to Quantum Dot Formation

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The controlled growth of semiconductor films can lead to the formation of nanometer-sized "quantum dots" which can provide enhanced optical and electronic performance in semiconductor devices. The standard approach for solving numerical simulations of this growth process, with the aim of understanding the important factors controlling quantum dot formation, is not efficient enough to permit large-scale or long-time simulations. Therefore, we implement a newly developed "unconditionally stable" numerical method for solving the equation. We proceed to investigate how to control quantum dot formation through tailoring the growth process to achieve a desired structure for a given material.

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Advanced simulations of photonic nanostructures

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A reliable simulation of optoelectronic devices requires a good understanding of numerous physical aspects. The analyzed device can be considered as an inhomogeneous system of carriers, which interact with themselves, the lattice and the optical field. While in some situations, the quantum properties of the carriers play the crucial role, in others they can be accurately described by classical physics. Commonly used approaches rely on classical models, often called the drift-diffusion approach. The main attraction of those models is the speed of calculations and the simplicity of incorporating physical effects. They are useful for researchers who need to get quick estimates of the characteristics of a design that is not too dissimilar from current designs. As the dimensions of semiconductor and optoelectronic (photonic) devices scale down to nano-scale dimensions (of the orders of hundreds of angstroms), kinetic and quantum effects in the carrier transport become crucial for the device's operation. In those circumstances, more fundamental approaches are necessary. Such approaches treat carriers as quantum many-body system with all possible interactions. The operation of active optoelectronic devices combines electrical transport of carriers along with optical field interacting with those carriers. In those devices spontaneous and stimulated emissions play an important role. To consistently describe spontaneous emission, the light field must also be quantized. The description of such carrier-photon system in principle is described by the many-particle Schroedinger equation. Our approach is based on non-equilibrium Green's functions (NEGF). The NEGF on a Schwinger-Keldysh contour will be introduced and all interactions incorporated by the self-energies. The total self-energy is the sum over the self-energies for each type of interaction so that they can be examined separately. Those self-energies for several types of interactions will be derived. The resulting Dyson equation is solved a self-consistent solution of with 1D Poisson equation. Our formalism allows to determine most important device parameters such as gain, spatial and spectral distributions of carriers and currents. One of the biggest disadvantages of conventional drift diffusion models is their high dependency on diffusion times and parameters which serve to broaden sharp peak of density of states (such as Lorentzian broadening). Our method allows to introduce many-body interaction corrections straight from microscopic theory which significantly reduces number of required phenomenological parameters.

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Minisymposium: Computational Number Theory

SS-CNT

Organizers:
Kevin Hare, *University of Waterloo (Canada)*
Patrick Ingram, *University of Waterloo (Canada)*

Many aspects of number theory have become active areas of research because of the advent of computers. Some examples include primality testing, elliptic curves, or calculations on L-functions. This session will discuss various aspects of number theory, and their relations to computers.

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Investigation of lower order terms in the moments of L-functions

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The problem of moments of L-functions has been the focus of intense research in recent years. Through the integration of random matrix theory and multiple Dirichlet series, methods for studying the moments of L-functions have been developed, leading to many well-posed conjectures for their asymptotics. A particularly interesting example involves the cubic moments of quadratic Dirichlet L-functions, where Diaconu, Goldfeld, and Hoffstein have conjectured the existence of an exceptional lower order main term, one which goes undetected via other methods. The possible existence of such exceptional lower order main terms in the moments of L-functions is a curious phenomenon and is one which will be investigated in this talk.

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On the Density of Abundant Numbers

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A natural number is classically defined to be abundant if the sum of its proper divisors exceeds the number itself. Davenport showed that the set of abundant numbers has a natural density, and Del'eglise determined the value of this density to the third decimal place, namely $0.247\ldots$. Recent improvements on the De'eglise algorithm have enabled the calculation of the fourth decimal place. We will describe these improvements, along with a new algorithm using the so called "primitive abundant numbers"; that compares favorably with Del'eglise's.

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Computing Irrationality Measures

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How close a real number can be approximated by rationals (with bounded denominators) is a question whose answer can tell us important information about the given number. This technique is often used to prove that numbers are transcendental, for example. If we restrict our attention to algebraic numbers then Roth's Theorem tells us how well the number can be approximated by an arbitrary rational number. However, the result is ineffective and hence not useful if our goal is to use the measure to derive tight bounds on the number of solutions to a particular Diophantine equation.

In this talk, we will discuss techniques for computing irrationality measures that are effective. By using Padè approximants to $(1-z)^{\nu}$ for rational ν, and an inordinate amount of luck, we can compute restricted irrationality measures for algebraic numbers of the form y^{ν}, for y fixed. The luck comes in finding one descent approximation to y^{ν} by searching over mediants of continued fraction convergents in the hopes of finding one such approximation with good non-archimedean properties.

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A proof of a conjecture concerning $\zeta(2j+1)/\pi^{(2j+1)}$

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We prove that some sets of polynomials have all of their zeros on the unit circle, a fact that was originally observed by numerical experiments. The polynomials are interesting because they have coefficients which involver Bernoulli numbers, Euler numbers, and the odd values of the Riemann zeta function.

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The Distance to an Irreducible Polynomial

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More than 40 years ago, P. Turán asked if every integer polynomial is 'close' to an irreducible polynomial. More precisely, he asked if there exists an absolute constant C such that for every polynomial $f \in \mathbf{Z}[x]$ there exists an irreducible polynomial $g \in \mathbf{Z}[x]$ with $\deg(g) \leq \deg(f)$ and $L(f-g) \leq C$, where $L(\cdot)$ denotes the sum of the absolute values of the coefficients. This problem remains open, and we report on some recent progress on it. By investigating the analogous question over certain finite fields, we determine that $C = 5$ suffices for all polynomials of degree at most 40, and we discuss how well our data fit the predictions of a heuristic model. We also show that one cannot obtain better results using the local strategy for large degrees, as we prove that a positive proportion of the polynomials in $\mathbf{F}_2[x]$ have distance at least 4 to any irreducible polynomial in this ring.

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Padé approximates and the Riemann Hypothesis

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Why look at the Padé approximants to the Riemann zeta function? The first reason, obviously, is the relationship to the Riemann hypothesis. Presumably, if one really understood any of the diagrams in these notes one would be able to prove the Riemann hypothesis. A worthwhile but rather too lofty goal.

But even assuming the Riemann hypothesis the particular behavior of the pproximations is not obvious. Clearly there is a limit curves both of the zeros and the poles. One goal is to figure out what these probably are.

It is harder than it looks to generate these pictures. Standard symbolic packages fail. So another part of the story is to describe the necessary computations.

There is a lovely body of theory due originally to Szegö that describes the zeros of the partial sums up the power series expansion of the exponential function. This extends to the zeros and poles of the Padé approximants to the exponential function and a few related functions. In order to get limit curves one scales the zeros and poles by dividing by the degree. The analysis is possible because there are explicit integral representations of the numerators and denominators.

There are no useful explicit representations known for the Padé approximants to the zeta function. Or even for the Taylor series. And indeed the principal problem in generating the approximations numerically is to derive large Taylor expansions.

This is the principal story that we want to tell in this paper. And to describe the computational difficulties that it involves.

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Vanishing theta nulls and genus 3 algebraic curves with automorphisms

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Let $\pi\colon \mathscr{X}_g \to \mathscr{X}_{g_0}$ be a m-sheeted covering of Riemann surfaces of genus g and g_0, where $g_0 \geq 1$. The general goal is to find properties that $\mathscr{X}_g$ (or rather, the Jacobian of $\mathscr{X}_g$) has, due to the existence of the covering π. This is an old problem that goes back to Riemann and Jacobi which is solved via the theta functions of the $\mathscr{X}_g$. Many other mathematicians have worked on the cases of small genus and small degree, most notably Frobenius, Prym, Königsberger, Rosenhein, Göpel, among others. In this paper we focus in the case when such covering is a Galois covering. More precisely, given an irreducible, smooth, algebraic curve $\mathscr{X}$ of genus $g \geq 2$ with non-trivial automorphism group $G := \text{Aut}\,(\mathscr{X})$; find relations of the theta functions of $\mathscr{X}$ which characterize the locus of curves with automorphism group G.

We give a brief review of basic definitions of theta functions and their $\frac{1}{n}$-periods. We define theta characteristics and theta-nulls for a given canonical homology basis. Furthermore, we briefly describe the group theoretic setup and the loci determined by group actions in $\mathscr{M}_g$. For a given group G and signature $\mathbf{C}$ the locus of curves of genus g is denoted by $\mathscr{M}_g(g,G,\mathbf{C})$ and is a subvariety of $\mathscr{M}_g$ (not necessarily irreducible). Finally, we give the list of groups that occur as full automorphism groups of genus 3 algebraic curves, their signatures, and the inclusions between the loci $\mathscr{M}_3(G,C)$.

Furthermore, we determine the decomposition of the Jacobians of genus 3 curves with automorphisms. This relates to the work of many authors and a conjecture of Serre on decomposition of Jacobians to elliptic components. As far as we are aware, this is the first time that such decompositions appear. In most of the cases the Jacobian completely splits into a product of elliptic curves. The decomposition of the Jacobians does not determine the locus $\mathscr{M}_3(G,\mathbf{C})$.

The list of automorphism groups of genus 3 curves and the inclusion among the loci $\mathscr{M}_3(G,\mathbf{C})$ is well understood; see [1][2] for details. Such loci are irreducible algebraic varieties in $\mathscr{M}_3$. The main goal of this paper is to describe such loci in terms of the theta-nulls. We first describe each case for non-hyperelliptic curves in terms of the half-periods and quarter-periods theta-nulls. The vanishing theta-nulls for hyperelliptic curves were studied by 19-th century mathematicians and are well understood. However, the non-hyperelliptic case is much more difficult. We focus on the curves with automorphisms and describe a strategy for genus 3 non-hyperelliptic curves in general.

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Mahler measures of elliptic curves

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The logarithmic Mahler measure of an n-dimensional Laurent polynomial is defined by

$$m(P) = \int_0^1 \dots \int_0^1 \log|P(e^{2\pi i t_1}, \dots, e^{2\pi i t_n})| dt_1 \dots dt_n.$$

Boyd conjectured many identities relating special values of Mahler measures, to values of L-series of elliptic curves. I will discuss recent progress on solving these conjectures. This is joint work with Wadim Zudilin.

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Tabulating All Cubic Function Fields via Class Field Theory

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Constructing algebraic number fields with certain properties is a central problem in computational number theory, as evidenced by the quite extensive body of literature on this topic. Research into the construction of certain low degree function fields has also surged in recent years, in part due to the cryptographic significance of elliptic and hyperelliptic curves. However there is comparatively little data available for higher degree function fields. This leaves open many questions about the number of non-conjugate function fields of fixed degree and a given discriminant, and even whether or not function field extensions of a given discriminant exist.

Tabulating lists of global fields is highly useful for analyzing statistics and identifying asymptotic behaviors. As such, they are essential to the formulation of hypotheses and conjectures, and are a valuable tool for providing support for or against the truth of important mathematical heuristics. For algebraic number fields there exists extensive tables for various degrees, some complete up to discriminants of 10^{11} or higher. However, outside of the case of quadratic function fields this valuable data barely exists in the function field setting.

In the particular case of tabulating cubic function fields there are only a few algorithms available, and like many algorithms for algebraic function fields they are often implemented first in a number field setting. In fact, the first real foray into this area is due P. Rozenhart [1] only a few years ago. He was able to generalize an algorithm of K. Belabas [2] from number fields to quickly tabulate certain cubic function fields. However, his technique only generates cubic fields of certain signatures and the discriminants are always square-free.

We will present an algorithm for tabulating a complete list of all cubic function fields over a fixed finite field of bounded discriminant degree. Our methods are based on those of H. Cohen [3] who tabulates cubic extensions of arbitrary number fields. The algorithm uses the tools of Kummer Theory and Class Field Theory, allowing for a natural transition to the function field setting. However, we are able to utilize the additional automorphisms of algebraic function fields to make significant improvements. Moreover, the algorithm is constructive in nature, allowing us to generate function fields of a specific discriminant as well. We will present the algorithm, our improvements, and the data we able able to generate. This will allow us to present the first true tests of various asymptotics.

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Some problems and results concerning Stern's diatomic sequence

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We will discuss some problems and results concerning Stern's diatomic sequence.

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Design and Analysis of Experiments & Statistical Methods

SS-DAE

Organizer:
Manohar L. Aggarwal, *University of Memphis (USA)*

The session will feature talks on all aspects of Design and Analysis of Experiments.

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Using LMS Algorithm for Estimating Gaussian Probability Distribution

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Evaluating integral of Gaussian Probability Distribution function $p(x)$ for arbitrary interval cannot be evaluated analytically and the value of the integral has to be looked up in a table. For the most part, the integral is computed either using analytical methods or using numerical approximation techniques. In this paper, we present a novel application which is based on the gradient method of parametric identification to estimate the probability of Gaussian distribution being in the range $[a,b]$ given by:$P(a \leq X \leq b)$.

A basic description of this method is to consider a periodic function of period greater or equal to $(b-a)$ and coincided with the Gaussian distribution function on the segment. This prolongation function, being periodic, can be developed in Fourier series. We then multiply the mean value by the interval to get the estimating probability . The method is implemented and tested on MATLAB for several intervals. Simulations results confirmed the numerical methods, and the error of estimation is highly dependent with adaptive algorithm. Furthermore, we note if the step-size is very small, then the convergence is slowly. But with a larger step-size, more gradient information is included in each update, and the convergence is more quickly; however, when the step-size is too large, the LMS algorithm will diverge. Finally, this method can be used for on-line applications.

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Maximum Likelihood Estimator for Parameters of Fractional Stable Distribution

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Fractional stable distributions (FSD) are limit distributions in the task of summation of independent identical distributed random variables X_j

$$S(t) = \sum_{j=1}^{N(t)} X_j \tag{2}$$

where $N(t)$ is the counting process $\sum_{j=1}^{N(t)} T_j \le t < \sum_{j=1}^{N(t)+1} T_j, T_j > 0$. Here random variables X_j belong to the region of normal attraction of Levy stable law with characteristic function $g(k;\alpha,\theta),\ (0<\alpha\le 2)$ and T_j belong to the region of normal attraction of one-sided Levy stable law with characteristic function $g(k;\beta,1),\ (0<\beta\le 1)$. The characteristic function of Levy stable law has the form $g(k;\mu,\theta) = \exp\left\{-|k|^{\mu}\exp\left(-i\frac{\pi\theta\mu}{2}\operatorname{sign}k\right)\right\}$, where $0<\mu\le 2$, $|\theta|\le \min(1, 2/\mu - 1)$.

In [1], it was shown that, on above assumptions asymptotic (at $t\to\infty$) distribution of the sum (2) is described by FSD

$$q(x;\alpha,\beta,\theta) = \int_0^{\infty} g(xy^{\beta/\alpha};\alpha,\theta)g(y;\beta,1)y^{\beta/\alpha}dy, \tag{3}$$

where $g(x;\alpha,\theta)$ is the strictly Levy law, whereas $g(y;\beta,1)$ is the one-sided strictly Levy law.

In the work the task of parameter estimation of distribution (3) is considered. Let $Y_1,\ldots,Y_N$ is sample of independent identical distributed random variables. Let distribution of each of them coincide with FSD (3) with characteristic parameters α and β. The task consist in estimation of a values $\hat{\alpha},\hat{\beta}$ of the parameters α and β by sample $Y_1,\ldots,Y_N$. For estimation of parameters the maximum likelihood method is used. Therefore, it is necessary to calculate the value of functional $\max_{(\alpha,\beta)} L(Y;\alpha,\beta) = \max_{(\alpha,\beta)} \frac{1}{N}\sum_{i=1}^{N} \ln q(Y_i;\alpha,\beta,0)$ for estimation of parameters α and β. Here $L(Y;\alpha,\beta)$ is logarithmic likelihood function. Monte Carlo method is used for estimation of FSD in the point Y_j. The algorithm of estimation of FSD by Monte carlo method was described in the work [2]. Using this results we obtain

$$\hat{L}(\alpha,\beta) = -\ln M + \frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{M}\ln\left[\frac{[S_j(\beta)]^{\beta/\alpha}}{\sqrt{4\pi S_j(\alpha/2)}}\exp\left\{\frac{Y_i^2[S_j(\beta)]^{2\beta/\alpha}}{4S_j(\alpha/2)}\right\}\right].$$

A further task consist in maximization value of this expression. In the speech it will be presented the results of parameter estimations for test samples. This work was supported by the Russian Foundation for Basic Research (project nos. 09-01-00815,10-01-00608).

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Robust Designs for Three Commonly Used Nonlinear Models

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In this paper, we study the robust designs for a few nonlinear models, including an exponential model with an intercept, a compartmental model, and a yield-fertilizer model, when these models are possibly misspecified. The minimax robust designs we considered in this paper are under consideration of not only minimizing the variances but also reducing the possible biases in estimation. Both prediction and extrapolation cases are discussed. The robust designs are found incorporating the approximation of these models with several situations such as homoscedasticity, and heteroscedasticity. Both ordinary and weighted nonlinear least squares methods are utilized.

First, we consider Model 1: $y \approx \beta_1 - e^{(-\beta_2 x)} + \varepsilon$. The robust designs for both prediction and for extrapolation are constructed and a comparison study with the classical optimal designs discussed by Ref. [2] is also presented.

Second, a compartmental model, previously discussed by Atkinson and Haines(1996) (see Ref. [1]), is revisited. We consider the construction of robust designs for its possible approximation: $y \approx e^{(-\beta_1 x)} - e^{(\beta_2 x)} + \varepsilon$, $\beta_2 > \beta_1$, for both prediction case and extrapolation case. The resulting robust designs are provided and we have observed that these designs in most situations considered are rather uniform.

Third, the robust designs for an approximate yield-fertilizer model (see Ref. [2]), $y \approx \beta_1 + \beta_2 e^{(\beta_3 x)} + \beta_4 x + \varepsilon,\ \beta_1 > 0$, $\beta_2 < 0$, $\beta_3 < 0$, $\beta_4 < 0$, is investigated under ordinary nonlinear least squares estimation with homoscedasticity. Since the estimate is a function of the model parameters, where it is $\hat{x} = \{\log(-\beta_4) - \log(\beta_2\beta_3)\}/\ \beta_3$, and thus c-optimal criterion is used.

In addition, we have also discussed the robustness of our designs against possible misspecification of the parameter values involved in the loss function due to nonlinearity. For instance, with Model 1, the resulting designs have very similar patterns for different β_2 values. With a greater β_2, the designs tend to be slightly more uniform and their high density regions tend to move a bit towards right.

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On simulating branching processes using mixed distributions

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The main aim of this paper is to study the behavior of mixed distributions in branching processes. We prove that the mixed distribution cannot effect on the number of particles in the nth period and it must be ignored for further simulations.

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Algebraic generation of Orthogonal Fractional Factorial Designs

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Generation of orthogonal fractional factorial designs (OFFDs) is an important and extensively studied subject in applied statistics.

In this talk we present a recent methodology [2], based on polynomial counting functions [1][3] and *strata*. This methodology allows to represent the OFFDs that satisfy a given set of constraints, expressed in terms of orthogonality between simple and interaction effects, as the positive integer solutions of a system Γ of linear equations.

We show how to use this system Γ

- to compute, for smaller cases, a minimal set of generators of all the OFFDs (Hilbert basis);
- to obtain, for larger cases, a sample of OFFDs.

Finally we describe a method to find minimum size OFFDs. We set up an optimisation problem where the cost function to be minimized is the size of the OFFD and the constraints are represented by the system Γ. Then we search for a solution using standard integer programming techniques.

It is worth noting that the methodology does not put any restriction on the number of levels of each factor and so it can be applied to a very wide range of designs, including mixed orthogonal arrays.

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Optimal and Robust Designs for Full and Reduced Fourier Regression Models

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The optimal and robust designs for Fourier regression models under different optimality criteria are discussed. First, we discuss the classical D-optimal designs for estimating pairs of coefficients and the classical Q-optimal designs for estimating the response function in a full Fourier regression model with a given order. Second, we investigate the minimax designs in case of Fourier approximation under A-, D-, and Q-optimality. We also demonstrate the equivalency of Q-optimal and A-optimal designs for Fourier regression in general. Third, the insensitivity of our resulting designs to a misspecified order of an assumed model is also discussed. Last, the D-optimal designs for some useful reduced Fourier models are constructed. Both the comparison study and simulation results show that the constructed designs incorporating the reduced models are efficient.

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Multilevel Hadamard Matrices

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Multilevel Hadamard Matrices (MHMs) have been examined by Trihn, Fan, and Gabidulin for constructions of multilevel zero?correlation zone sequences, which in turn have useful application in quasi?synchronus code division multiple access (CDMA) systems. Subsequently, Adams, Crawford, Greeley, Lee and Murugan introduced a construction of full?rate circulant MHMs that proved the existence of an order n MHM with n elements of distinct absolute value for all n. We examine MHMs, the family of full?rate circulant MHMs (FCMHMs) introduced by the construction of Adams et al. and explain the existence of other forms of FCMHMs by means of new constructions.

AMMCS-2011

Evolutionary Games in Biology and Ecology

SS-EG

Organizers:
Joe Apaloo, *St. Francis Xavier University (Canada)*
Ross Cressman, *Wilfrid Laurier University (Canada)*

Evolutionary game theory was initially developed almost forty years ago by the biologist, John Maynard Smith, to predict individual behavior in biological systems withour explicitly modeling the dynamics underlying their behavioral evolution. Nonetheless, the theory has been used to successfully characterize the dynamic stability of many such models. Recent examples include the Darwinian dynamics approach that combines behavioral evolution with evolving population sizes and the adaptive movements methods that investigate the spatial distributions of species among multiple habitats. The session will feature research advances in these topics as well as in other areas of game theory applied to biology.

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Stability in Models of Behavioral and Population Coevolution: Time Scales in Predator-Prey Systems

Ross Cressman[1]

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Coevolution of behavior (or strategy) structured populations is often analyzed by separating the time scale of behavioral evolution from that of population dynamics. For instance, the canonical equation of adaptive dynamics studies the evolution of the population mean strategy assuming that fast population dynamics instantaneously track stable equilibrium densities for the current strategy. In other models of coevolution (e.g. habitat selection models), it is more realistic to assume that behavioral changes act much faster than the density dynamics. The talk will discuss stability of equilibria in both of these extremes as well as for models that do not assume a separation of time scales. In particular, the theory will be applied to predator-prey structured-population systems.

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Neighborhood Invader Strategies in Co-evolutionary Models

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Static stability criteria which combine to ensure the stability of an evolutionary dynamic in single species evolutionary models with strategies drawn from a continuous trait space are well established. Considering the stability of the singular points of these evolutionary models, and the manner in which they are approached, three main static stability criteria have been very useful: ESS, convergence stable, and NIS. A concrete result is that a singular point that is an ESS and neighborhood invader strategy is also convergence stable, and that an ESS combined with convergence stable or NIS ensures the stability of the evolutionary dynamic. This result has not been established generally for multispecies evolutionary models due to lack of necessary multispecies static convergence stable and NIS criteria. Several static criteria for multispecies evolutionary games with particular emphasis on NIS will be presented.

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Strategic effects of mobility in predator-prey systems

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In this paper we investigate the dynamics of a predator-prey system with the assumption that both prey and predators use game theory-based strategies to maximize their per capita population growth rates. The predators adjust their strategies in order to catch more prey per unit time, while the prey, on the other hand, adjust their reactions to minimize the chances of being caught. Numerical simulation results indicate that, for some parameter values, the system has chaos-like behavior. Our investigation reveals the relationship between the game theory-based reactions of prey and predators, and their population changes.

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Species coexistence in non-ESS communities: It's all about NIS (Neighborhood Invasion Stability)

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A convergent stable, ESS community of coexisting species is special. It is not so diverse as to result in the exclusion of any of the coexisting species, yet it is diverse enough to prevent the invasion of any other species into the community. But, when the species do not possess the strategies of the ESS, then quite different communities are possible, some not as diverse as the ESS others actually more diverse. For instance in a community with just a single species at a globally stable ESS, it is possible for two species to coexist so long as there is a peak (or a valley) of the adaptive landscape between them. And this ESS must be more than just convergent stable, it must also be NIS. That is the strategy of the ESS can invade not only each species in isolation (by definition of the NIS) but the pair of species as they coexist. This means that for two species to coexist around the peaks of an ESS, the ESS must lie between the two strategies. This property seems to hold for ESSs with more than one species. If each peak has the NIS property, then up to two times as many species as the ESS can coexist when the community is not at its ESS. We conjecture that for vector-valued strategies, the number of coexisting species around a peak of an ESS can be as many as one plus the dimension of the strategy vector. This may have more than just abstract significance. With human disturbance many communities may no longer possess species at their ESS. This leave open the possibility of species invasions which may either result in species replacement, or, if NIS, then the coexistence of resident and invader species on opposite sides of the actual ESS.

AMMCS-2011

Recent Advances in Energy Harvesting Technologies

SS-EHT

Organizer:
Armaghan Salehian, *University of Waterloo (Canada)*

In today's world troubled with all the energy crises, technologies which harvest, employ and store ambient energy have received much attention in recent years. Wind turbines, solar batteries, solar cells and magneto-vibrating energy harvesting devices are examples of these technologies. Research concerning hybrid techniques for harvesting energy which employ applications of smart materials will be highlighted in this special session, but submissions pertaining to general area of energy harvesting techniques are welcome.

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Modeling and Evaluation of a Hybrid Piezo-Electromagnetic Vibrating Energy Harvesting Device

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The efficiency of mobile electrical devices increased over the last years. Self-supply by harvesting ambient energy became a possibility of reducing operational costs by ruling out the need of battery replacement.

Many energy harvesting devices employ cantilever configurations with base excitation to increase the effective displacement. The proposed design extends this design with an electromagnetic harvesting device (EMH) placed at its tip. It features an alternating stack of magnets with opposing poles and discs of highly permeable material. The composite cylinder is encircled by coils. This EMH design has successfully been employed for ocean wave harvesting and vehicle suspension systems. Its efficiency with respect to mass and energy output is compared to a previously published design using a single magnet placed at the tip moving within a coil.

There exists proof that combining readily available technologies into a so-called coupled or hybrid design can increase the efficiency in comparison to respective stand-alone designs. Once the model for the proposed design is derived and evaluated, it will be extended by a piezoelectric harvesting device at its base.

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Horizontally-Aligned Springless Energy Harvester

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Energy harvesting is the process of extracting energy from ambient sources and converting it into electrical energy. Vibration based energy harvesters (VEH) use mechanical oscillators and transducers, such as electromagnetic, piezoelectric, and electrostatic, to collect kinetic energy from ambient vibrations and transform it into electrical power. The center frequency of the VEH is determined by the spring stiffness coefficient k and the effective mass m. This limits VEH to frequencies larger than $10-15\,\text{Hz}$.

In this paper, we examine a proposed springless electromagnetic VEH that can harvest energy from ambient vibrations at a very low center frequency $< 15\,\text{Hz}$. The harvester consists of an electromagnetic transducer, a carriage carrying the magnets and the seismic mass along a linear guide, and two end-stops to limit the carriage motion. The carriage and magnets move freely along the linear guide with respect to a stationary surface coil in response to base excitations. The motion of the carriage induces a voltage V across the coil terminals.

In this final manuscript, we will present a mathematical model of the horizontal electromagnetic VEH, estimate its parameters experimentally, and present experimental and simulation results of the VEH performance.

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Thermally-robust Asymmetric Resonators for Energy Harvesting Applications

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Energy harvesters are systems that derive energy from external sources, e.g., ambient vibrations, capture and store it for other autonomous systems, e.g., wireless sensors networks. Resonators are the building block of vibration-based energy harvesters. The challenge in the design of these resonators is matching their resonance frequency with the environment frequency of vibration. For instance, the frequency of vibration of a bridge can change from warm days of summer to cold days in winter, however, the resonance frequency of the resonator may not change similarly, because of different thermal expansion coefficients. In addition, a vibration source may contain several peaks in its frequency spectrum. To fully exploit the available energy, either several different resonators, or a single resonator with several resonance frequency must be used.

In this paper, we propose using one asymmetric resonator [1] for energy harvesting. An asymmetric resonator is a clamped-clamped beam with an attached, which can be a permanent magnet or an electrostatic transducer. Instead of using a simple fixed end, we use a set of chevron short beam to clamp the beam at one end.

We employ finite element models to demonstrate that 1) the resonance frequencies of the resonator can be adjusted by setting the location of the attached mass on the beam and its rotary inertia, 2) the mode shapes of vibration can be accommodated to achieve adequate vibration displacement of the attached mass at each desired frequency, and 3) the thermal sensitivity of the resonance frequencies of the resonator can be tailored by designing proper length, thickness, and angle of chevron beams with respect to resonating beam [2].

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AMMCS-2011

Homogenization and Applications in the Modeling of Nanoplasmonic Sensors

SS-HAM

Organizer:
Chitra Rangan, *University of Windsor (Canada)*

Gold and silver nanoparticle and nanofilm sensors are the next generation of technologies for chemo and bio sensing. These sensors are based on 'plasmonics' - the study of collective charge excitations at the interface of a metal (such as gold) and dielectric (such as glass or water) that are excited by light. The mathematical modelling of such systems involves the homogenization of Maxwell's electromagnetic wave equations in the presence of metal nanostructures arranged in two or three dimensions within a dielectric matrix. The complex dielectric function of the metal nanostructures added to the numerous configurations yield a rich variety of solutions that will be explored in this session.

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Dispersion Engineering Nano-scale, Light-Steering Devices

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Dispersion engineering is a general methodology for designing optical materials in which the constituent elements and geometry are tailored to select allowable modes, or electromagnetic oscillations, in a material's microstructure and to model their microscopic flow. An optical material is designed by selecting the constituent components and geometry of the material's microstructure, using electromagnetic solvers to find the modes sustained within the microstructure and the coupling strengths between the modes, and then refining the components and geometry of the microstructure based on the results of the solvers. The end result of this iterative process is a blueprint of a microstructure that sustains a set of propagative modes that confine light along a pre-determined pathway. We will describe the application of dispersion engineering to design a suite of nano-scale devices capable of light-bending, light-trapping, and broadband resonance. The potential application of these materials for biosensing, solar conversion, and optical circuitry will be discussed.

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Analysis of Coherent Interactions in 2-D Gold Nanoparticle Arrays based nanoplasmonic sensors

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Localized surface plasmon resonance (LSPR) characteristics of gold nanoparticles can be utilized to design highly sensitive label-free nano-sensors [1]. The large extinction cross-sections of gold nanoparticles render them very sensitive by inducing large wavelength shifts of the LSPR peak in response to a change in the refractive index in the surrounding medium. In sensor applications, this refractive index change in a surface bound layer typically is typically induced by binding of biomolecules, chemical reactions or phase transition of polymers hence allowing detection of these events. Of particular interest is the large tunability of the LSPR of gold nanoparticles by changing the shape and size of the particle, and also by the coherent interactions of periodic arrays. Solid gold nanoparticles exhibit visible LSPR while gold nanorings, split-rings and nanocrescents show LSPR in the near-infrared spectral range.

Here we present our studies on 2-D periodic array of gold nanoparticles in a square lattice configuration on top of the glass substrate using finite difference time domain (FDTD) simulations. The parameters of interest are the trends in LSPR peak positions and the sensitivity of the peak shift and peak width. The sensing figure of merit (defined as sensitivity divided by peak width) is found to be significantly affected by the lattice constant of the array. In the evanescent grating order range, the coupling of the periodic array causes strong peak sharpening effects and enables the figure of merit to be greatly improved [2]. To gain comprehensive knowledge on the effects of coherent interactions on the sensing characteristics, we have studied the effects from two different types of substrates, one with a thin absorptive layer on top (ITO-coated glass) and the other one as low loss substrate (Pyrex substrate) and different shapes of nanoparticles including gold nanodots, nanorings and split ring structures. An increase in sensitivity and figure of merit is observed for arrays over single nanoparticles or random ensemble of particles. This indicates the coupling the gold nanoparticles is strongly affected by the optical properties of the substrate and the periodic array interactions. This study can potentially provide guidance in the design of the 2-D periodic gold nanoparticle arrays for highly sensitive sensors.

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Effective Media Parameters for Dielectric Based Metamaterials

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Artificial materials often referred to as metamaterials have been a subject of intense research in the past few years. Although the term metamaterial is sometimes misused to refer to devices such as electronic and microwave filters, in its proper usage, metamaterials are collections of scattering elements that are often but not always arranged on a periodic lattice. A signature of metamaterials is the fact that the dimensions of inclusions and periodicities are at least an order of magnitude smaller than the operating wavelength. In this sense, metamaterials have their roots in the well know and celebrated effective medium theory in which the microscopic properties of the underlying scattering elements (atoms and molecules in the case of "real materials" and meta-atoms and meta-molecules in the case of metamaterials) are expressed in terms of effective macroscopic properties such as effective permittivity, permeability, or index of refraction.

Undoubtedly, recent interest in metamaterials and effective media was rekindled by Smith' experimental observation of Veselago's theoretical prediction that an overlap of frequencies for which the real parts of both permittivity and permeability are negative would lead to observation of a negative index of refraction. Although the original experiment by Smith and consequent work by others utilized metallic scatterers; however, presence of metallic structures and conduction currents are not a necessary conditions for negative permeability, permittivity, and index of refraction. In fact, it has been shown by our group that both negative permeability and negative index of refraction can be observed in polaritonic dielectrics such as SiC. Our presentation begins with a brief overview of the metamaterials. It will be shown how inclusion of dielectric scatterers in a host medium can lead to the observation of an effective permeability at infrared (IR) frequencies and how by coating the inclusions one can obtain negative index of refraction at these frequencies. Next, a sample of random shape and size dielectric scatterers is considered and experimental evidence indicating the presence of a magnetic response at IR will be presented. To explain this experimental observation a theoretical model which includes the effects of size and shape variations of the scattering elements will be developed. Next, a simple coupled dipole model and a more sophisticated method of exact multiple scattering via T-matrix will be used to investigate the effects of coupling among the scatterers. To test the predictions of the aforementioned theoretical models the results of an experiment with a linear chain and a ring composed of dielectric spheres at microwave frequencies will be discussed. Lastly, a method to retrieve the general effective medium tensors of periodic metamaterials, which does not generate any unphysical implications, will be presented. The primary result is an algorithm to extract the complete polarizability tensors of a single isolated inclusion based on its scattering properties. These polarizabilities are properties of the inclusion, and remain valid for any arrangement of such inclusions. The remainder of the problem is the abstract homogenization of the microscopic polarizabilities into the macroscopic effective medium parameters. This de-coupling of the microscopic and macroscopic aspects of the problem allows one to choose the most appropriate effective medium model.

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Metallic nanoparticles on waveguide structures: Effects on waveguide mode properties, and the promise of sensing applications

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Surface plasmon polaritons, waveguide modes, and other such electromagnetic field excitations bound to a surface or to a multilayer structure are signalled by poles in the Fresnel coefficients of reflection and transmission. We consider a waveguide structure overcoated with metallic nanoparticles, either in an ordered array or randomly distributed, with the size of the particles and the distances between them small compared to the wavelength of light. The presence of the nanoparticles will modify the "self-wavenumber" of the waveguide mode, in general adding a real part associated with a shift in wavenumber, and an imaginary part associated with absorptive loss. We develop a simple strategy for calculating these shifts and decay rates. Image dipoles in the medium below the cladding make an important contribution to properties of the structure, so a homogenization strategy cannot be implemented for the nanoparticles alone; it must be done in the presence of the waveguide structure. Nonetheless, the problem can be simplified and reduced to one where at most a numerical calculation is necessary to treat only longitudinal electric fields; transverse field components can then be included in an analytic way because they vary little over nanoparticles and the distances between them, and we treat them with a simple transfer matrix formalism. Since in the plane of the nanoparticles the longitudinal electric fields are short-range, the required numerical calculation is not problematic. As an even simpler first step we consider the limit of nanoparticles treated in the point dipole approximation, where everything can be done analytically. This allows for a first exploration of the use of such structures in sensing applications, where the properties of the waveguide mode, already modified by the presence of the nanoparticles, will be modified again by adsorbed species or a change in the optical properties of the cladding. We find that nanoparticle-covered waveguide modes offer a number of interesting possibilities for sensing applications.

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Minisymposium: Recent progress on hybrid dynamical systems

SS-HDS

Organizer:
Xinzhi Liu, *University of Waterloo (Canada)*

Hybrid dynamical systems exhibit both continuous and discrete dynamical behavior and have attracted a growing interest of researchers around the globe in recent years due to their important applications in various industrial and technological areas such as communication, complex networks, biotechnology, artificial intelligence, switching circuits in power electronics, spacecrafts control, and ecosystems management. This minisymposium intends to provide an opportunity to learn and share new developments and to present research results in the theory and applications of hybrid dynamical systems.

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Preservation of dissipativity properties with the (θ, γ)-discretization

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In this talk we deal with complementarity dynamical systems, with possible state jumps, and extensions of these in the class of multivalued Lur'e dynamical systems. In view of the state of the art on time discretization of such nonsmooth systems, higher order methods are not yet available and only first order methods (implicit or explicit Euler, Paoli-Schatzman's scheme ([1]) have been shown to converge.

The problem that we tackle is as follows:

Given an extended θ- discretization method (referred to as the (θ, γ)-discretization), find the class of continuous-time dissipative systems such that their discretized counterpart is still dissipative with the same storage (energy) function set, supply rate (reciprocal variables) and dissipation function.

Our results consist of classifying the various forms of preservation conditions, as well as clearly characterizing 'what is' numerical dissipation, with examples on switched circuits.

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Observer for Singularly Perturbed Switched Linear Time−Varying Systems

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Recently, considerable effort has been put in the study of switched systems and, hence, the problem of obtaining full state information for control and diagnostic purposes has become an active research area. Also, there are many man-made or natural singularly perturbed systems in control, finance, and power systems. The main contribution of this paper is to develop an observer for time-varying linear singularly perturbed systems. Typically, a linear switched systems with N singularly perturbed modes has the form

$$\begin{aligned} \dot{x} &= A_{11_i}(t)x + B_{11_i}z, \\ \varepsilon_i \dot{z} &= A_{12_i}(t)x + B_{12_i}z \\ y &= C_1(t)x + C_2(t)z, \end{aligned}$$

where x, z and y are the slow state, fast state, and output vectors, respectively. Also, for all $t \in \mathbb{R}_+$ and $i = 1, 2, \cdots, N$, $A_{11_i}(t), B_{11_i}(t), A_{12_i}(t), B_{12_i}(t), C_1(t)$, and $C_2(t)$ are time-varying matrices with proper dimensions. ε_i is a small positive parameter. Based on this system an observer is proposed which can estimate all system states. Moreover, the stability and convergence of the state error system is investigated through the selection of an appropriate Lyapunov function and Lyapunov theorem.

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Stability Results for Nonlinear Stochastic Impulsive Systems with Time Delay

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Impulsive systems have been studied extensively by numerous researchers in recent years. Such systems belong to a class of hybrid system whose states undergo abrupt changes. The duration of these changes are often negligible when compared to the total duration of the process, so that they can be reasonably approximated as instantaneous changes of the states or as impulses.

In this work, we establish some stability results in the Lyapunov sense for stochastic impulsive systems with time delay (SID). Particularly, we use Razumaikhin technique. In the first part of this work, we show that when impulses occur at fixed times and its total effect is bounded, it is guaranteed that the trivial solution of the SID is stable in the pth-moment provided that the corresponding non-impulsive system is stable in the pth-moment. Moreover, under similar conditions on the impulses, it is uniformly asymptotically stable in the pth-moment if the corresponding non-impulsive system is uniformly asymptotically stable in the same probabilistic sense.

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Controllability and Observability of Linear Time-Varying Impulsive Systems on Time Scales

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The theory of time scales was initialed by Stefan Hilger in his Ph.D. thesis in 1988 [1], with the express purpose of unifying continuous and discrete analysis. It provide a framework for us to handle both continuous and discrete systems simultaneously.

In this talk, we shall review the basic theory of time scales (for more details about time scales, refer to [2-4]) and formulate the problem of linear time-varying impulsive systems on time scales. Several sufficient and necessary criteria for state controllability and observability of such systems will be given and these criteria will be compared with the existing results. It is shown that the classical results about controllability and observability problems of linear continuous impulsive systems can be generalized to the impulsive systems on time scales. Moreover, as the integers $\mathbf{N}$ being a kind of time scale, our results can reduce to the corresponding results of linear discrete impulsive systems, which, to the best of our knowledge, have not been investigated.

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Intermittent Impulsive Synchronization of Coupled Chaotic Systems Subject to Delay

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In this paper, intermittent impulsive synchronization of coupled chaotic systems is studied, subject to time delay. In reality, there usually exist some uncontrollable periods in the synchronization process due to some practical restrictions such as distance limitation, cost limitation, etc. When these uncontrollable periods are larger than the upper bound of impulsive intervals in impulsive synchronization process, general impulsive synchronization scheme does not work well any more. To deal with this challenging problem, we present a new novel synchronization scheme, called intermittent impulsive synchronization scheme. In our scheme, impulsive control is only activated in the control windows, rather than during the whole time. Several criteria for chaos synchronization are established, utilizing the method of linear matrix inequalities (LMI) and Lyapunov-Razumikhin theory. In the end, a numerical example is given to demonstrate the effectiveness of the analytical results.

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Designing Stochastic Adaptive Impulsive Observer for Noisy Uncertain Nonlinear Impulsive Systems

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State observation (estimation) is a very important issue in system analysis and control. A vast amount of literature focuses on giving different approaches for state estimation of nonlinear, stochastic, uncertain, or time-varying systems. On the other hand, in nature and industry, a large class of systems are subject to impulsive effects. However, the state estimation of impulsive systems is not investigated thoroughly. Generally, a nonlinear stochastic impulsive systems with uncertainties has the form

$$\begin{aligned} dx(t) &= [Ax(t)+f(x(t))+h(x(t))\theta+Bu(t)]dt+g(x(t))dw(t), \qquad t\neq t_i \\ \Delta x(t^+) &= I(t,x(t)), \qquad t=t_i \\ dy &= Cx(t)dt, \end{aligned}$$

where $x(\cdot), y(\cdot), u(\cdot)$ and θ are the system state, output, input, and unknown parameter vectors, respectively. Also, $f(\cdot), h(\cdot), g(\cdot)$, and $I(\cdot,\cdot)$ are smooth vector functions. $w(\cdot)$ is a standard Brownian motion, and it models the system noise which is inherent in any practical system. This work presents a new observer called Stochastic Adaptive Impulsive Observer, which is applicable to the aforementioned system.

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Stability of stochastic switched SIRS models

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In the real world, epidemic models are often affected by environmental noises and the presence of a noise source can modify the behavior of corresponding deterministic evolutions of the systems [1, 2].

In this talk, stochastic switched epidemic SIRS models with or without time delay are constructed and investigated. Utilizing the stochastic stability theories about the stochastic differential equations with Markovian switching in [3] and the Lyapunov methods, sufficient stability conditions of the disease-free equilibrium of the associated epidemiological model are obtained. The results show that it is not necessary to require every subsystem of the stochastic switched epidemic system be stable, but as the result of Markovian switching, the overall behavior maybe stable. Finally, numerical simulations are presented to illustrate our mathematical results.

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Stabilization of a class of nonlinear hybrid systems using state-dependent switching and impulsive control

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Switched systems, which are types of hybrid systems, evolve according to mode-dependent dynamics and experience abrupt changes between modes, triggered by threshold events. Recently there has been a wide interest in the study of hybrid systems, as they have applications in many diverse areas such as control engineering, mechanical systems, computer science, robotics, secure communications, and biological systems. For an unstable system where continuous control is not suitable or cannot be found, it may be possible to use switching control to stabilize the system. Further, as many systems exhibit impulsive effects at switching times, impulsive control, in combination with switching control, can be used as a powerful stabilization tool. Motivated by the many practical applications of switched systems, the objective of this work is to design state-dependent switching strategies that guarantee stability of nonlinear hybrid systems by using switching and impulsive control. Discrete and distributed delays, which are important in applications like neural networks and epidemic models, are also considered. Some state-dependent switching rules are carefully chosen so that the switched systems have a strictly decreasing Lyapunov function (or functional). From this, some sufficient conditions can be determined which guarantee stabilization. Finally, some simulations and future directions are given.

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Invariance Principles for Hybrid Systems: Review and New Results

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As demonstrated by the celebrated LaSalle's principle, invariance principles can characterize asymptotic stability of nonlinear systems in the absence of strict Lyapunov functions. Due to the many important applications of hybrid dynamical systems, invariance principles for hybrid systems are particularly useful. However, for hybrid system models, the classical versions of invariance principles cannot be applied. In this paper, we review and establish new invariance principles for hybrid systems, emphasizing systems with time-delays, impulsive effects, and possible stochastic disturbances. Applications of these invariance principles are illustrated by practical examples arising from neural networks, population dynamics, and epidemic models.

AMMCS-2011

Minisymposium: High Order Numerical Methods for Partial Differential Equations

SS-HONM

Organizers:
Ching-Shan Chou, *The Ohio State University (USA)*
Jun Jia, *Oak Ridge National Laboratories (USA)*
Yulong Xing, *University of Tennessee and National Oak Ridge Laboratories (USA)*

Many processes in science and engineering can be described and formulated by partial differential equations. In recent years, there has been vast development in high order numerical methods for solving these equations. This minisymposium aims to bring together researchers from various fields to report the progress in numerical PDEs that addresses computational challenges arising from complex physical systems, geometries, high dimensions, etc. The focus is on new high order algorithms that will impact diverse areas such as fluid mechanics, kinetic simulations and math biology. The numerical methods presented in our minisymposium range from discontinuous Galerkin method, WENO scheme, spectral method, finite volume method to deferred correction method.

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High order AMR based on WENO

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In this talk we introduce a high order adaptive mesh refinement method. The method is based on combining 5th order finite difference weighted essential non-oscillatory (WENO) methods and TVD RK3 with an AMR methodology in such a way as to maintain 5th order in space and third order in time. The new approch is applied to a series of challenging 1D and 2D problems and is show to have better performance then low order AMR based.

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Robust reconstructions for unstructured WENO schemes

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The weighted essentially non-oscillatory (WENO) schemes are a popular class of high order numerical methods for hyperbolic partial differential equations (PDEs). While WENO schemes on structured meshes are quite mature, the development of finite volume WENO schemes on unstructured meshes is more difficult. A major difficulty is how to design a robust WENO reconstruction procedure to deal with distorted local mesh geometries or degenerate cases when the mesh quality varies for complex domain geometry. In this talk, I will present our recent work on combining two different WENO reconstruction approaches to achieve a robust unstructured finite volume WENO methods on complex mesh geometries. Numerical examples including both scalar and system cases, and application to a biological problem will be shown.

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High order, stable numerical simulations of rigid-rod nematic polymers

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The kinetic model equations for rigid-rod nematic polymers are extremely expensive to simulate numerically because of the orientational configuration of the polymer at every spatial position. Due to the effect of coupled long range distortional elasticity and short range excluded volume potential, it is desirable to utilize a stable and efficient numerical method to solve the model equations. Spectral deferred correction (SDC) method for ordinary differential equations has been developed and studied in the past decade. It can produce higher order numerical solutions through successive corrections. It also exhibits certain desirable stability properties. In this talk, I will show how the SDC method is used in the simulations of rigid-rod nematic polymers. We first discretize the spatial variables and use the method of lines to get a large system of ODEs and then the SDC method is performed on the resulting ODEs. Some evidences will be given to show the effectiveness and the stability of the SDC method in our simulations. Then various numerical simulation results about the structures of rigid-rod nematic polymers are carefully examined, including the elasticity dominated steady state, the viscous dominated steady state, the wagging state, and the composite tumbling-wagging state. The defect core will also be studied.

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High-order positivity-preserving DG-FEM for Vlasov models of plasma

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Vlasov systems describe the evolution of a collisionless plasma represented through a probability density function (PDF) that self-interacts via electromagnetic forces. There are several difficulties in solving Vlasov systems: (1) the high-dimensionality of the system (3+3+1), (2) the severe time-step restriction that arises from parts of the PDF associated with moderate-to-large velocities, and (3) the need to accurately conserve various physical quantities (i.e., mass, momentum, and energy). The dominant approach in the plasma physics community is the so-called particle-in-cell (PIC) method, which discretizes the distribution function into a set of macro-particles, while the electric field is represented on a mesh. We develop in this work grid-based alternatives to PIC by discretizing phase space via high-order discontinuous Galerkin (DG) methods. A major aim of this project is to explore several efficient time-stepping strategies that can be generalized to a variety of settings: Vlasov-Poisson, Vlasov-Maxwell, and relativistic Vlasov-Maxwell. In all cases we design positivity-preserving limiters. These approaches are tested on several test cases.

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Augmented High Order Finite Volume Element Method for Elliptic PDEs in Non-smooth Domains: Convergence Study

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The accuracy of a finite element numerical approximation of the solution of a PDE can be spoiled significantly by singularities. This phenomenon is especially critical for high order methods. For example, the solution of the Poisson equation with analytic right hand side and boundary conditions in a unit square domain is smooth enough for the first order finite element approximation to attain an optimal order of convergence using the Galerkin Finite Element Method (FEM). On the other hand, since the unit square domain has four right angle corners, it can potentially have second derivative blow up singularities which make the solution not smooth enough to have an optimal rate of convergence for the quadratic finite element approximation.

Thus, in order to take full advantage of high order finite element approximations, it is essential to have an efficient strategy to deal with such singularities. One of the strategies to avoid this decay of the convergence rate is the augmentation of the trial function space. The idea of augmentation of the trial function space for the FEM using results from regularity analysis can be found in Grisvard as well as in Strang and Fix. Although it has been shown that the augmentation of the trial function space can recover the optimal convergence rate of the FEM, additional singular basis functions in the trial function space introduce complications. Integration of the singular basis function must be done analytically or using special quadrature rules, and special care is needed to preserve the sparsity of the stiffness matrix.

In this talk, we show that, if the PDE is linear and the singular basis functions are homogeneous solutions of the PDE, the augmentation of the trial function space for the Finite Volume Element Method (FVEM) can be done significantly simpler than for the FEM. The FVEM is a numerical method for approximating the solution of a partial differential equation in a trial function space spanned by piecewise polynomial basis functions, similarly to the Finite Element Method. The coefficients of the linear combination of the basis functions are obtained by imposing the PDE through integrations over control volumes, similarly to the Finite Volume Method. Recently, Vogel et al. have constructed a high order FVEM using arbitrary high order piecewise polynomial basis functions.

When the trial function space is augmented for the FVEM, all the entries in the matrix originating from the singular basis functions in the discrete form of the PDE are zero, and the singular basis functions only appear in the boundary conditions. That is to say, there is no need to integrate the singular basis functions over the elements and the sparsity of the matrix is preserved without special care.

As examples, we present convergence studies for the Poisson equation in an L-shaped domain with a reentrant corner. We first show that the rate of convergence of the high order FVEM is reduced due to the singularity. In particular, as we will show the convergence plot in the presentation, no matter how high the order of the method is, the convergence rate in the H1 error norm cannot exceed order 2/3. However, by augmenting the trial function space with singular basis functions, we recover the high order convergence of the high order method.

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A discontinuous Galerkin solver for front propagation with obstacles

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We are interested in front propagation problems in the presence of obstacles. We extend a previous work (Bokanowski, Cheng and Shu, SISC, 2011), to propose a simple and direct discontinuous Galerkin (DG) method adapted to such front propagation problems. The DG scheme is motivated by the variational formulation when the Hamiltonian H is a linear function, corresponding to linear convection problems in presence of obstacles. The scheme is then generalized to nonlinear equations, written in an explicit form. Stability analysis are performed for the linear case with Euler forward, a Heun scheme and a Runge-Kutta third order time discretization using the technique proposed in Zhang and Shu (SINUM, 2010). Several numerical examples are provided to demonstrate the robustness of the method. Finally, a narrow band approach is considered in order to reduce the computational cost.

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High-order of approximation method for modeling of aerodynamics of flapping wings

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The numerical model of aerodynamics of flapping airfoils in generalized pitching motion has been developed. Non-inertial coordinate system combined with high-order compact approximation in space and high-order scheme in time was used. Comparison of numerical results for pitching and plunging motion of airfoil with the experimental data at Re=10000 showed good agreement for the stream-wise velocity and vorticity, wake velocity profile, and streak-lines. The pure pitch case was considered for the pitching axis located at different points along the chord. It was observed that the maximum mean coefficient of lift was obtained when the pitching axis was at the leading or trailing edge. The comparison of the CFD results with the quasi-steady expressions showed a good agreement between them. The momentarily lift appears to be order of magnitude higher than steady lift caused by the angle of incidence; however, the time-averaged value of lift is only moderately higher than that for steady flight. Then, the generalized pitching motion was studied for three different phase differences between the pitching amplitude and the motion of the axis. It was found that the use of quasi-steady approximation leads to significant error in the estimate of lift coefficient and therefore CFD computations are essential for the generalized pitching motion of wings. It was found that the maximum mean coefficient of lift was produced when the phase difference was 90 degrees. Further, the value of lift was found to be more than doubled compared to that obtained by combined pitch-plunge motion. However, unlike the combined pitch-plunge motion the generalized pitching motion did not produce thrust. Finally, a modified kinematic motion which adds a plunging motion to the generalized pitching motion was investigated. It was found that this superposition of the motions increased the value of the lift coefficient compared to a generalized pitching motion. Further, it also generated thrust force as opposed to the generalized pitching motion. Findings of this study support the use of superposition of complex kinematic motions to obtain a needed amount of lift and thrust.

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High Order Krylov deferred correction methods

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In this talk, we present Krylov deferred correction methods for accurate and efficient time-integrations. The methods treat a collocation formulation using spectral deferred correction techniques as preconditioners, where the collocation is equivalent to the quadrature based implicit Runge-Kutta method. The preconditioned nonlinear system is then solved with Newton-Krylov schemes. The resulting Krylov deferred correction (KDC) methods for ODE can be of arbitrary but finite order of accuracy and A-stable. The methods are applied to solve the 2-D shallow water equations with th climate dynamics core HOMME. The stability and accuracy properties are compared to the previous time-stepping methods in HOMME.

AMMCS-2011

Minisymposium: High Performance Computing: From Models of Computation to Applications

SS-HPC

Organizers:
Marc Moreno Maza, *University of Western Ontario (Canada)*
Yuzhen Xie, *University of Western Ontario (Canada)*

Topics of this special session includes theoretical tools (cache complexity, multithreaded parallelism, space-time tradeoffs, code optimization for parallelism and locality, etc.) that are adapted for taking best advantage of parallel architectures and hierarchical memories. Applications of these models in all areas of mathematical sciences and reports comparing implementation techniques of a given algorithm on different hardware architectures (multicores, GPGPUs) would also be of great interest.

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Exploiting the GPU for Multiple Swarm Collaborative PSO for Task Scheduling Cloud Environment

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A significant problem in a heterogeneous distributed computing environment, such as grid/cloud, is the optimal matching of tasks to machines so as to utilize the resources efficiently to minimize the overall execution time. Task matching becomes computationally intensive as the number of tasks and machines increase. Many heuristic algorithms exist for the task mapping problem. More recently, bio-inspired heuristic algorithms such as Particle Swarm Optimization (PSO) (Ref. [1]) have been used and studied for this problem (Ref. [2]). The nature of algorithms such as PSO, potentially allows for the generation of improved solutions without significantly increasing the costs associated with the matching process.

The basic PSO algorithm, as described by Kennedy and Eberhart (Ref. [1]), works by introducing a number of particles into the solution space (a continuous space where each point represents one possible solution) and moving these particles throughout the space, searching for an optimal solution. In the literature, single swarm PSO has been applied to the task matching problem. Recently, Vanneschi (Ref. [3]) proposed an algorithm that uses multiple swarms and a repulsive factor on each particle in a swarm to avoid stagnation at a local optima. We propose a modification of this algorithm for the task matching problem.

In recent years, GPUs have provided significant performance improvements for many parallel algorithms. As the GPU offers a tremendous level of parallelism, our experiments show that multi-swarm PSO provides a good fit for the architecture. With a greater number of swarms, and, thus, a greater number of particles, we can make better use of the threading capabilities of the GPU. Our results show that the GPU offers a high degree of performance and achieves a maximum of 37 times speedup over a sequential implementation when the problem size in terms of tasks is large and many swarms are used.

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Solving Bivariate Polynomial Systems on a GPU

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We present a CUDA implementation of dense multivariate polynomial arithmetic based on Fast Fourier Transforms (FFT) over finite fields. Our core routine computes on the device (GPU) the subresultant chain of two polynomials with respect to a given variable. This subresultant chain is encoded by values on a FFT grid and is manipulated from the host (CPU) in higher-level procedures, for instance for polynomial GCDs modulo regular chains.

We have realized a bivariate polynomial system solver supported by our GPU code. Our experimental results (including detailed profiling information and benchmarks against a serial polynomial system solver implementing the same algorithm) demonstrate that our strategy is well suited for GPU implementation and provides large speedup factors with respect to pure CPU code.

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Determinant Computation on the GPU using the Condensation Method

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Dodgson's Algorithm for computing the determinant of a square matrix A of order n is a popular trick among students. It is, indeed, much easier to perform by hand on paper than the other classical methods (minor expansion, Gaussian elimination). This is due to its amazing data traversal patterns. Dodgson's Algorithm can be executed as a stencil computation: the input data array is transformed into n successive data arrays. Each transformation step (from one array to the next one) is a streaming process, called a condensation. This suggests that this algorithm is a good candidate for an implementation within a concurrency platform based on data-parallelism such as CUDA.

Dodgson's Algorithm suffers, however, from a serious algebraic limitation: it may fail to compute the targeted determinant. Indeed, after each condensation, the newly generated matrix should have no zero elements in its interior [1] for the next condensation step to take place. One can sometimes reduce to this case by combining rows or columns. When this is not possible, then the algorithm terminates without producing any answers.

In [2], the authors have solved this difficulty by introducing another type of condensation, which we summarize. The input is a square matrix A of oder $n > 2$. If the first row of $A = (a_{i,j})$ is the null vector then the determinant of A is zero and the process stops. Otherwise, let ℓ be the smallest column index of a non-zero element in the first row of A. The condensation step produces a matrix $B = (b_{i,j})$ of order $n-1$ defined by:

$$b_{i,j} = \begin{vmatrix} a_{1,\ell} & a_{1,j+1} \\ a_{i+1,\ell} & a_{i+1,j+1} \end{vmatrix}$$

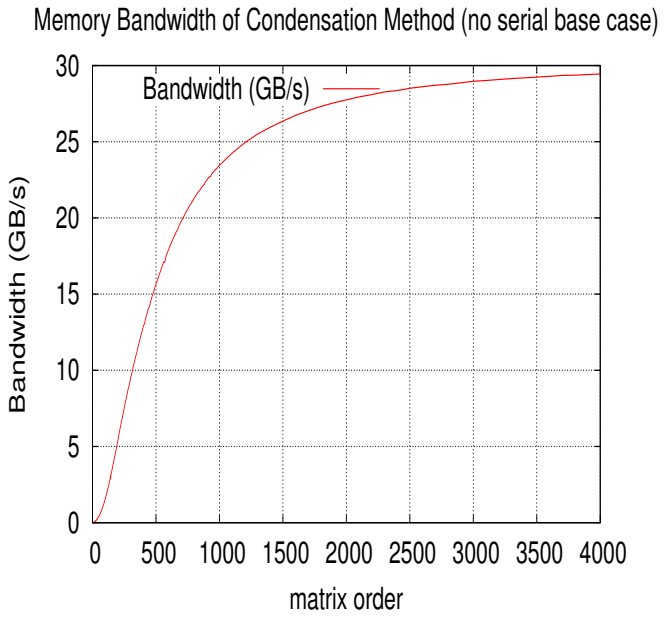
for $j \geq \ell$ and by $b_{i,j} = -a_{i+1,j}a_{1,\ell}$ for $j < \ell$. The key relation between A and B is the following:

$$\det(A) = \det(B)/(a_{1,\ell})^{n-2}.$$

We have realized a CUDA [6] implementation of the Algorithm of Salem and Said for matrices with coefficients in Z/pZ where p is a prime number of machine word size. Each condensation step is performed by one kernel call and the termination test (checking the first row of the condensed matrix B) is performed by this kernel too.

We have applied our code to compute the determinants of random square matrices. We vary the order of the square matrix from 10 to 4000. We compare our code with NTL [3] and Maple [4] counterpart functions. The comparison of computing times of our GPU code with Maple and NTL code are shown in Figures. We also report on the effective memory bandwidth of our GPU code.

These results show that, for matrices over finite fields, a GPU implementation of a condensation method can outperform optimized CPU implementation of Gaussian elimination methods, despite of the higher (essentially by



a factor of 2) algebraic complexity of the former method. Our effective memory bandwidth results show that our code is reasonably efficient (but could be further improved) since the maximum memory bandwidth of our card (Tesla 2050 C) is 96 GB/s.

One could have expected that for n small enough, a host code should relay the device code, due to low occupancy on the device. Experimentation (not reported here) shows that this is not the case. It is possible to conduct the entire determinant computation on the device while preserving competitiveness with respect to pure CPU code for $n \geq 80$. For smaller values of n, transfering the data back to the host (for continuing the computations there) is not worth.

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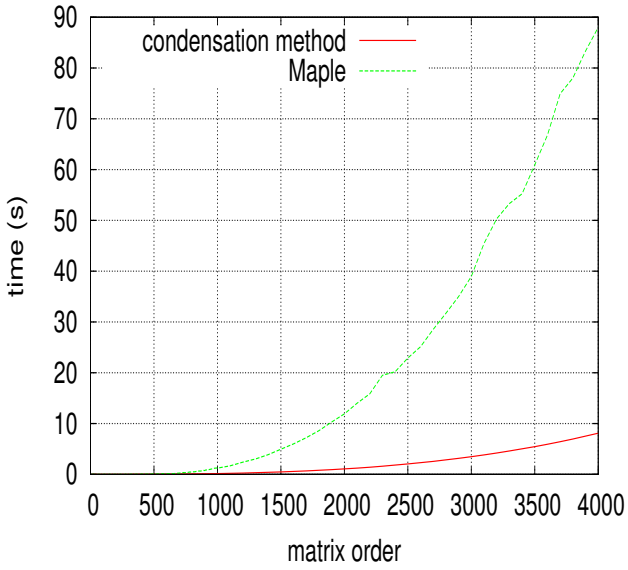
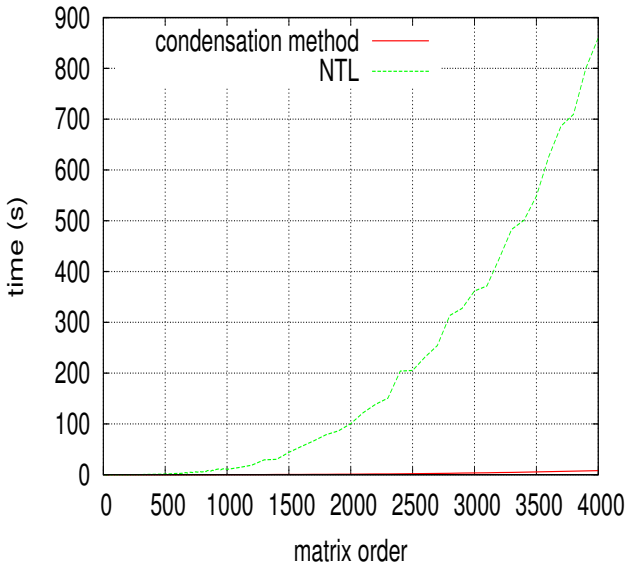
Condensation (no serial base case) Vs Maple code for computing determinant



Condensation (no serial base case) Vs NTL code for computing determinant



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Parallel evolutionary algorithms, for solving a free boundary problem.

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This paper deals with an inverse heat conduction problem, modeling a welding process. It consists in finding the temperature distribution in the solid part and the weld pool. This described by the following optimal design problem.

$$\begin{cases} \text{find } \Omega^* \in \Theta_{ad} \text{ solution of} \\ J(\Omega^*) = \inf_{\Omega \in \Theta_{ad}} J(\Omega) \\ \text{where } J(\Omega) = \dfrac{1}{2}\displaystyle\int_{\Gamma_0} |T(\Omega) - T_0|^2 \, d\sigma \\ \text{and } T(\Omega) \text{ the solution of} \\ (SP) \begin{cases} \mathcal{V}_0 \cdot \nabla T = \nabla \cdot (\lambda \nabla T) + f \text{ in } \Omega \\ \lambda \dfrac{\partial T}{\partial \nu} = 0 \text{ on } \Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \\ T = T_d \text{ on } \Gamma_4, \quad T = T_f \text{ on } \Gamma, \end{cases} \end{cases} \tag{1}$$

where Ω is the solid part, Γ is the weld pool (free boundary), $\mathcal{V}_0$ is a torch velocity, λ is the thermal diffusivity of the solid part, f is a given source term. The quantities T_d, T_0 and T_f are given temperatures. Θ_{ad} denote the set of admissible domains.

To solve this problem we investigate the efficiency of various evolutionary algorithm based on genetic algorithm combined with fuzzy logic. These algorithms combine the notion of survival of the fittest with evolutionary operators to form a robust search mechanism. The parallel version of this algorithms combined with the fuzzy logic Controller to form a hybrid methodologies is tested and compared and proved particulary promising. The numerical tests presented demonstrate the computational advantages of discussed methods.

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Grappling with Garantuan Graphs of Neural Functional Connectivity.

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Functional magnetic resonance imaging (fMRI) allows for the direct visualization of cerebral bloodflow, which has been demonstrated to correlate very strongly with neural activity (see, e.g., [1]). Neuroscientists have recently begun employing network-theoretic tools to discover patterns of functional and structural connectivity within the brain. In the case of studying functional connectivity, one maps voxels in regions of interest onto graph vertices and, if the underlying fMRI time series between two such voxels have a similarity (measured using, e.g., Perason correlation, spectral coherence or mutual information) exceeding some threshold, one places an edge between the respective vertices in the graph. With neural "functional similarity" converted into graph form, one may apply classic graph and network theoretic metrics both to quantify intrinsic neural functional networks and to attempt metric-based classification problems such as detecting disease states.

Most prior work on such graphs has been undertaken with a small number of seed "regions of interest" (ROIs) manually specified by the investigators and, indeed, the most popular toolkit for this type of analysis, the *Brain Connectivity Toolbox*, is a set of MATLAB^{TM}scripts that place limitations on the sizes of the networks that may be handled. It has recently been demonstrated that even small errors in the selection of ROIs can have major consequences on the reliability of the generated network [2] and we have thus undertaken to develop a software toolchain capable of generating, and analyzing, whole-brain networks. This approach is fully data-driven and eliminates any possibility of error introduced by suboptimal ROI selection as the entire brain becomes the ROI.

In this talk we will outline the challenges faced in developing the tools, and theory, required to analyze brain graphs with tens of thousands of nodes and potentially hundreds of millions of edges and discuss the neuroscientific insights gained by the use of these tools. On the technical side we will compare results from full-size graphs processed on the novel, and ideally suited to graph problems, Cray XMT architecture with results from smaller SMP clusters using reduced-size graphs. This will include a discussion of graph size reduction, using the new technique of metrically-constrained graph minors. We discuss also a protocol optimization process in which we compared several graph-theoretic metrics, and several methods of graph generation, on fMRI data to determine which metrics are "orthogonal" and which are statistically recapitulating results accessible with computationally less-complex metrics allowing us to suggest an optimal, and computationally minimal, set of metrics.

Finally, we will present preliminary results of the application of our tools to real fMRI data and the new scientific insights gained, including an insight into the pseudo-hierarchical organization of prefrontal cortex.

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High-Performance Parallel and Stream Processing of X-ray Microdiffraction Data

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High-brilliance synchrotron X-ray microbeams combined with fast large-area two-dimensional detectors can produce large blocks of X-ray microdiffraction (XRD) data at unprecedented rates. In principle, up to 1 to 10 images per second of 8MB in size can be produced. This allows scientists to study crystalline texture in polycrystalline materials using Polychromatic X-ray Microscopy (PXM), and has led to refinements that permit the mapping of crystallographic orientation and strain deviation of such materials. Even at this early stage, such measurements involve the accumulation of data sets as large as 60,000 4MB images. Using even advanced desktop computers it would take several days to index the diffraction patterns produced using software such as XMAS (X-ray Microdiffraction Analysis Software) developed at the Advanced Light Source and the 3D X-ray Microdiffraction Analysis Software Package at the Advanced Photon Source. An advance on this software was FOXMAS that uses cell processors to accelerate the process by a factor of up to 15.

In this paper we report on the development of a software system for analyzing synchrotron white-beam Laue diffractions using parallel and stream processing on clusters of off-the-shelf multi-core processors: today's mainstream architectures. Stream processing is a data-centric programming model. Given a set of data which can be structured as a stream of tuples, a series of operations (processing elements) are applied to each tuple or some set of tuples in the stream. Processing elements are usually pipelined, much like an assembly line. Pipelining does not reduce the time for individual instruction execution, but instead, it improves instruction throughput. Our implementation platform is the IBM InfoSphere Streams. InfoSphere Streams enables the development and execution of applications that process information in data streams. It provides built-in operators as well as a programming interface for end-users to create user-defined operators to operate on data streams. The runtime system and the scheduler of InfoSphere Streams help to seamlessly deploy stream applications to clusters of multi-core processors.

Based on the three software packages mentioned above, we revisit the crystallographic principles of Laue diffraction and its mathematical model (using Vector Algebra) and present an overview of the implementation techniques used for our stream processing implementation. We first re-engineer the sequential procedures for processing images individually in order to optimize the code and improve memory usage. We then adapt the algorithms and restructure their memory access patterns for parallel and stream processing. As a result of these techniques, our software is about ten times faster than the sequential C program used in FOXMAS to process a single image. On a quad-core desktop, super-linear speedup is obtained for processing four images by four pipelines. With the support of the runtime system and the scheduler of InfoSphere Streams, our software is able to be scaled up to operate on clusters of multi-core processors. It serves as a high-performance processing kernel that can be used to achieve near real-time data analysis for synchrotron experiments, the ultimate goal of the Active Network Interchange for Scientific Experimentation (ANISE) project.

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Complexity and Performance Results for Non FFT-Based Univariate Polynomial Multiplication

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Today's parallel hardware architectures and computer memory hierarchies enforce revisiting fundamental algorithms which were often designed with algebraic complexity as the main complexity measure and with sequential running time as the main performance counter. This study is devoted to two algorithms for univariate polynomial multiplication algorithms that are are independent of the coefficient ring: the *plain* and the Toom-Cook univariate multiplications. We analyze their cache complexity and report on their parallel implementations in `Cilk++`.

AMMCS-2011

Industrial Mathematics

SS-IM

Organizers:
Sean Bohun, *UOIT (Canada)*
Huaxiong Huang, *York University (Canada)*

Industrial problems challenge mathematicians in ways not common to the standard academic environment. A number of such problems will be discussed in this special session.

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Worst case analysis for deterministic online algorithm in capacitated lot-sizing problem

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It is essential to realize that optimization of production planning process is a significant issue in manufacturing and it is based on mathematical modeling and optimization algorithms. However, in practice it is quite often impossible to know demands for a certain product in advance. This is precisely the case when industrial and scientific interests come across in analyzing this issues and developing robust solutions for them. In this paper the robust optimization is considered, which allows to get the solution with guaranteed quality under incomplete information about demands.

The most important objectives of introduced research include: to analyze a capacitated lot-sizing problem (CLSP) on a rolling horizon basis, to prove the uniqueness of worst-case demand distribution in terms of competitive analysis, to construct a method to calculate a competitive ratio of online algorithms with different length of rolling horizon interval.

To describe the process of production, mathematical model of CLSP was chosen (includes associated production and holding costs) (see Ref. [1]). In this paper we consider the rolling horizon approach for the optimization. We propose that demand is known only for n periods through the overall planning horizon $N, (n < N)$. Rolling horizon algorithm provides the optimal solution for known planning horizon n, but only plan for the first planning period is fulfilled. Then the model is updated with a new data and solved again. Such kind of algorithms are called online as they receive input data in parts, which can lead to non-optimal solution for an overall planning horizon. To measure the effectiveness of the algorithm and guarantee the robust solution, we use terms 'online and offline algorithms' and the concept of competitive ratio from competitive analysis (see Ref. [2]).

After the problem definition and mathematical model description, several assumptions were formulated. It allowed to analyze the influence of different demand distributions on the value of competitive ratio. Based on several crusial assumptions, the theorem, which defines the worst-case of demand distribution was formulated and proved. To illustrate the theorem statement, a small computational example was considered. In turn, proved worst-case demand distribution allowed to formulate the method of calculating the competitive ratio for deterministic online algorithm with an arbitrary planning interval.

In addition, interesting directions for the future research exist in this field, e.g. the case when only borders for the corresponding demand interval or possible percentage demand changes are given.

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Radiation Dose Planning and Portfolio Management

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The idea of radiation therapy for cancer treatment is to direct radiation to damage a tumor while avoiding surrounding healthy tissue. Because dose delivery cannot be exactly shaped to the tumor, this procedure has inevitable tradeoffs. The biology of cancerous vs. healthy tissue may, to a crude degree at least, be approximated by a so called linear-quadratic model. An optimization problem results which we cast in terms of a dynamic program and solve to give two different optimal dose delivery programs (fractionation schedules) as a function of input biological parameters.

However, the input parameters to this problem are not known with certainty and may, in fact, fluctuate over time. We analyse our optimal solution in this light and find that, under the uncertainty, it becomes very hard to beat a very simple equal dose per fraction schedule.

This problem and its results bear many similarities to results from the theory of financial portfolio optimization, and some of the parallels will be exposed in this talk.

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Understanding buoyant miscible displacement flows in near horizontal ducts I.

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In many oilfield operations one fluid displaces another along a long duct, (pipe or annulus), e.g. drilling, cementing, fracturing. Often the fluids are miscible, the ducts are typically inclined, the fluids may be Newtonian or non-Newtonian, and density differences are common. We study the simplest meaningful situation of 2 miscible iso-viscous Newtonian fluids, and consider laminar displacements at duct inclinations close to horizontal, where the heavier fluid displaces the lighter fluids. Through a mix of semi-analytical models, 2D numerical simulation, lab-scale experiments and dimensional analysis we are able to identify 5-6 different characteristic flow regimes and use the simpler semi-analytical models to give quantitative approximations of the front velocity of the displacement, which in turn gives the displacement efficiency.

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Finite element approach for numerical simulation of advection-diusion equation

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This paper presents numerical solution of advection diusion equation us- ing B-spline nite element approach. We use cubic B-spline functions with least square formulation which gives numerical results very close to the solutions avail- able in the literature. Some test problems are studied to validated the algorithm. Main advantage of this technique is that the algorithm is very simple and is easy to implement.Dierent comparisons are made with some of the existing numerical schemes and analytical solutions. Excellent agreement with the other solutions is observed.

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Model and simulations of the Gao beam with a crack

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This talk presents, analyzes, and simulates the dynamics of a Gao beam that may come in contact with a reactive foundation, and which has an evolving symmetric edge crack. The problem is set as a variational inequality coupled with a differential equation for the evolution of the damage variable, which measures the severity of the crack. The existence of a local weak solution for the model is shortly discussed using approximations, and a priori estimates. A finite element scheme for the problem is proposed,and representative simulations presented. In particular, the dependence of the beam's vibration frequency on the crack's position and size is depicted.

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Numerical model for Magnetized Target Fusion

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[2] *Carleton University*

Controlling the energy released by thermonuclear fusion is considered one of the 21^{st} century Grand Challenges. General Fusion, a start-up from Burnaby in BC, proposes to achieve fusion through a compression process entitled MTF. The plasma, contained in a sphere of liquid lead, is compressed by a strong acoustic wave created by the mechanical impact of pistons. In partnership with General Fusion, the researchers propose a numerical model of the early stages of compression of this complex device. The Frontier and Pluto codes are used and some of the key issues are the interface between the lead and the plasma and the energy transfer between the pistons and the plasma target.

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The Augmented Lagrangian Method Applied to Unsolvable Power Flows

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This paper aims to present and discuss a new and robust approach to restore the network electric equations solvability. The unsolvable power flow is modeled as a constrained optimization problem. The cost function is the least squares of the real and reactive power mismatches sum. The equality constraints are the real and reactive power mismatches at null injection buses and/or at those buses that must have their power demands totally supplied for technical or economical criteria. The mathematical model is solved using an algorithm based on Augmented Lagrangian methods considering the particular structure of the problem. The inner iterations of the proposed methodology are solved using Levenberg-Marquardt (LM) algorithm. Numerical results for both IEEE test systems and a real equivalent system from the Brazilian South-Southeast region are presented in order to assess the performance of the proposed approach.

AMMCS-2011

Large scale computer algebra applications

SS-LSCA

Organizer:
Thomas Wolf, *Brock University (Canada)*

From its beginning, computer algebra was developped to perform large symbolic computations which are not possible by hand. What one would describe as 'large' today are computations which require to work with a large amount of data, say > 100 GB, or computations which take very long, say >1 week on one CPU, or omputations that are rich, needing many different algorithms and programs to work savely together over extended periods of time, or computations which show all these features.

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A Unified Sampling Scheme for Fast Approximation of the Multiplication of Several Matrices

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Motivated by several sampling schemes, several algorithms from [1,2,3] and a conditional sampling algorithm from [4], we propose a unified sampling scheme for approximating the multiplication of several matrices.

We give the theoretical analysis on the error bound of our algorithm. Based on the analysis of the influence of sampling rate on the trade-off between the accuracy and efficiency of the algorithm, we propose a method for adaptive choice of sampling rates given the error tolerance.

Experimental evidences suggesting the superiority of our method are also presented. We show the practical application of proposed method on the computation of dominant eigenvector by estimating the power of matrix, an example of product of several matrices. Compared with power iteration approach, which is traditional to compute the dominant eigenvector, our method outperforms in terms of accuracy with comparable efficiency.

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Cache Complexity and Multicore Implementation for Univariate Real Root Isolation

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Isolating the real roots of a univariate polynomial is a driving subject in computer algebra. This problem has been studied under various angles from algebraic algorithms to implementation techniques. Today, multicores are the most popular parallel hardware architectures. Beside, understanding the implications of hierarchical memory on performance software engineering has become essential. These observations motivate our study. We analyze the cache complexity of the core routine of many real root isolation algorithms namely, the *Taylor shift*. Then, we present efficient multithreaded implementation on multicores. In some cases, our implementation fully utilizes the memory space of a 32-core cluster node allowing to tackle problems that are out reach for a desktop implementation.

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A solver for large sparse linear algebraic systems

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The study of integrability of non-abelian Laurent ODEs includes the computation of symmetries, first integrals and Lax-pairs. Using the method of undetermined coefficients the computational tasks include the solution of polynomial algebraic systems that are either non-linear and involve a few hundred variables or that are linear but very large. A specialized solver for large sparse and overdetermined linear systems has been developed that was able to determine the general solution of systems with over a billion equations for 170 million variables.

After an introduction to the subject and a description of the challenges the methods used in the computation will be explained and results be discussed.

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AMMCS-2011

Minisymposium: Recent Advances in Mathematical Biology

SS-MB

Organizers:
Sue Ann Campbell, *University of Waterloo (Canada)*
Yuming Chen, *Wilfrid Laurier University (Canada)*

Mathematical Biology uses mathematics to understand and solve complex problems in many fields of biology and medicine including Ecology, Epidemiology, Oncology and Neuroscience. In recent years, a better understanding of the relevant problems and emerging issues in these fields have led to new advances in Mathematical Biology research. This session will provide an opportunity for participants to exchange and share experiences and research results, and discuss the potential challenges for future work.

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A Coupled Plankton System with Instantaneous and Delayed Predation

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We present two simple plankton population models, one has instantaneous predation, another has delayed predation. The models consist of two coupled differential equations representing the interaction between phytoplankton and herbivorous zooplankton with additional effect of zooplankton predation by a constant fish population. We study the dynamical behavior and investigate the conditions to guarantee the coexistence of two species, address the stability and bifurcation under different density of fish, with or without the maturation time delay. Analytical methods and numerical simulations are used to obtain information about the qualitative behavior of the models.

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Bifurcation of Canard Cycles in Predator-Prey Competition Models

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There have been extensive stability and bifurcation studies of classical predator-prey models[3][4], yet the study of canard cycles of such type of model is rather limited due to the technical difficulties. By using the techniques introduced by Dumortier and Roussarie about center manifolds and singular perturbation [1][2], we study the bifurcations of canard cycles in a general singular perturbed predator-prey model, and apply the results to obtain canard cycles in the model with different Holling types of functional responses.

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The dynamics of a laissez-faire model with two predators

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In this talk, I present the dynamics of a laissez-faire predator–predator–prey model with specialist and generalist predators. I analyze the stability of equilibria by performing linearized stability analyses. I reexamine the stability of the equilibrium where the prey and predator coexist by constructing a Lyapunov function. If I hold the generalist predator population constant, treating it as a bifurcation parameter, I show that the model can possess multiple limit cycles that surround an equilibrium in the interior of the first quadrant. My model shows rich dynamics including fold, transcritical, pitchfork, Hopf, cyclic-fold, and Bautin bifurcations, as well as heteroclinic connections. If I instead vary the generalist predator population slowly across bifurcations, the model exhibits bursting behavior as it alternates between a repetitive spiking phase and a quiescent phase.

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Mathematical Modeling of Cancer Cell Metabolism

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The metabolism of cancerous cells is significantly different from that of normal cells, and hence there has been much research dedicated to the development of drugs that target specific metabolic pathways in malignant tumors. In addition, conventional cancer therapies and advanced molecularly targeted treatments can directly or indirectly affect cancer cell metabolism. Hence, a deeper understanding of cancer metabolic pathways and their interactions with various treatment strategies is required before they can be successfully translated into clinical practice.

To determine the exact cell metabolism of cancerous tissues, we have recently proposed a novel theoretical approach based on micrometer scale measurements of the concentration of nutrients and other chemical species as functions of distance from a single blood vessel [1]. In this talk, after a brief introduction, we will discuss the method and its application to available experimental data [2]. We will show how the model can be used to determine the exact in vivo cell metabolism for malignant tumors. In addition, the model will be used to derive mechanisms responsible for the lack of correlation between hypoxia and acidity in solid tumors. Finally, we will discuss the application of the model in the study of the effect of cancer treatments on the tumor microenvironment and cancer cell metabolism.

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A Differential Equations View On Honeybees, Varro Destructor And The Deadly Viruses That They Carry

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A famous folklore quote, commonly but most likely wrongfully attributed to Albert Einstein says that four years after honeybees disappeared from the Earth, mankind will disappear too. The message is clear: no bees, no pollination, no food, no people. Recent years have seen honeybees in distress, with up to 35% of colonies breaking down annually. The causes of this phenomenon, sometimes refered to as Colony Collapse Disorder, are not well understood. Among the least disputed stressors for bees are the parasitic varroa mites and the deadly viruses that they carry. Focusing on the Acute Bee Paralysis virus, we present a simple ODE model for the honeybee-mite-virus complex, which we study with analytical and computational techniques.

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Early vaccination against HSV-2

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Genital herpes is one of the most incident and prevalent sexually transmitted infections in the world. Currently, candidate vaccines against HSV-2, the main cause of genital herpes, are in various stages of clinical trial. If any of these vaccines, or a future one, is approved to be administered to the population. it is imperative that an effective vaccination program be determined. We have developed a mathematical model to describe the dynamics of HSV-2 disease in a population, including a vaccination strategy targeting 13 year old girls. The vaccination program is similar to one that is already in place for HPV. We delineate the population by age, sex and sexual behaviour. Results show that this vaccination program is effective in reducing HSV-2 prevalence, however, this highly depends on the proportion of girls vaccinated, the age of sexual maturation, and the immunogenecity of the vaccine (whether it prevents infection or disease). Eradication is very hard to achieve.

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How generation-based insights can inform antibiotic stewardship

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Many infectious diseases are caused by parasites that multiply within their hosts. The size and composition of the parasite population will change as the immune response escalates, when drug treatments are prescribed, and as the host resources needed for parasite replication are depleted. When hosts are prescribed antibiotics, parasite strains that are antibiotic resistant may emerge. These strains survive longer, reproduce more, and are increasingly likely to be transmitted to other hosts.

For a simple scenario where: (i) only two types of antibiotics are available; (ii) a life history trade-off constrains parasite strains to be resistant to one antibiotic or the other; (iii) treatment is certain to select for the emergence of resistance, and (iv) all new infections are generated on the T^{th} day of the infection, a simple strategy, 'generation rotation', ensures that antibiotics are always administered to hosts with a sensitive strain of the infection. For this simple scenario, how many previous hosts the parasite has infected (the generation of the infection) can be determined because new infections always occur after a fixed duration. 'Generation rotation' treats all infections of a given generation with the same antibiotic, and since resistance is certain to emerge and a life history trade-off exists, then all infections in the next generation will be sensitive to the other antibiotic.

The 'generation rotation' strategy is optimal for the simple scenario described above and maximizes the chance that the next infected host is treated with a different antibiotic. Previous work states that maximizing heterogeneity in drug treatments explains why certain antibiotic prescription strategies outperform others (Ref. [1]). In this talk, I will identify the assumptions needed for the heterogeneity principle to hold and will discuss how the principle can practically be applied given that infection spread is stochastic and many different generations of infection may coexist simultaneously.

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Analyzing heterogenous transmission dynamics of infectious diseases: an integrated approach to the Lyapunov functions

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With more complex structures added to epidemiological models to describe transmission heterogeneity of infectious diseases, analyzing dynamical behaviors of these systems pose a great changlleage for applied mathematicians and modelers.

Motivation from HIV/AIDS modeling is presented and earlier development of Lyapunov functions and recent progress in this area are briefly recalled. Based on the graph-theoretical approach recently developed, I will introduce the integrated approach to the method of Lyapunov functions and its application to a large class of epidemic models with complex compartmental structures.

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Epidemiological Effects of School Cohort Entry

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Changes in transmission rate associated with school terms accounts for the well-known biennial pattern of measles incidence observed in the pre-vaccine era in many places. However, the discontinuity of school admission (school cohort entry effect) has usually not been modelled explicitly. In this paper, we show that the school cohort entry effect alone can explain the biennial pattern. Furthermore, a model with seasonal forcing from both school terms and cohort entry fits measles data better than a model with either one of the effects alone. In addition, the model with both effects yields the most plausible estimate of the basic reproductive ratio.

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Modelling behaviour-incidence dynamics: the impact of social contact structure and social learning

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Infectious disease transmission models have a relatively long history, with modern origins dating to the early twentieth century. Traditionally in such models, the level of use of an infectious disease intervention–such as the percentage of the population that receives antiviral therapy–has been treated as a fixed model parameter, under the implicit assumption that a central decision-maker has more or less unlimited ability to set the level of use of infectious disease interventions in the population. However, in many cases, "policy resistance" means that the response of the system to the introduction of an intervention has a nontrivial impact on the level of use of the intervention in the population. For instance, under a voluntary vaccination policy, as vaccine coverage climbs, the individual incentive to vaccinate starts to decrease as herd immunity makes the infection more rare. This may result in suboptimal vaccine coverage, or the population may exhibit a disproportionate response to small vaccine risks–a vaccine scare. Mathematical models that capture the nonlinear feedback loop between disease transmission and individual vaccinating behaviour are increasingly studied. These may take the form of ordinary or delay differential equations, network models, or other spatial models, with assumptions about human behaviour being based on game theory or some other psychologically motivated theory. The predictions of such models can vary dramatically depending on how transmission is modeled and what assumptions are made about human behaviour. I will discuss some of these issues and present some recent work using approaches from evolutionary game theory to capture behaviour-incidence dynamics in a system of ordinary differential equations. I will also attempt to address the question of whether such models are actually of any use in predicting or understanding real-world behaviour-incidence dynamics. Such models may eventually become helpful tools for policy-makers who wish to understand or predict the response of a human system to the introduction of a new vaccine or the emergence of new data on vaccine risks. This work is joint with Samit Bhattacharyya.

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Robust control underlying the bacterial growth laws

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In bacteria, the rate of cell proliferation and the level of gene expression are strongly interdependent. Elucidating these relations is important both for understanding the physiological functions of endogenous genetic circuits and for designing robust synthetic systems. We have recently described a phenomenological study that reveals intrinsic constraints governing the allocation of resources toward protein synthesis and other aspects of cell growth (Ref. [1]). A theory incorporating these constraints can accurately predict how cell proliferation and gene expression affect one another, quantitatively accounting for the effect of translation-inhibiting antibiotics on gene expression and the effect of gratuitous protein expression on cell growth. The use of such empirical relations, called *bacterial growth laws*, may facilitate our understanding and manipulation of complex biological systems before the details of the underlying regulatory circuits are known.

The most striking feature of these growth laws is their linearity ([1]), despite the millions of highly nonlinear and strongly coupled chemical reactions that must occur during each doubling of the bacterium. I will briefly outline the bacterial growth laws, then turn attention to the complex regulation that underlies protein synthesis and cell growth. I will demonstrate how very simple control functions for the allocation of the protein synthesis machinery of the cell can give rise to the observed behaviour.

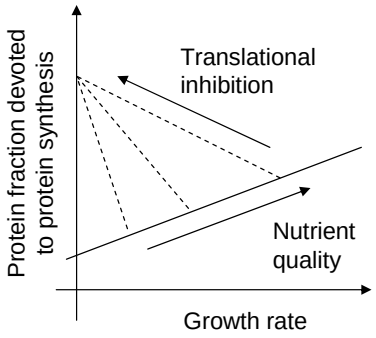

Figure 1: With growth rate modulated by changes in nutrient quality (solid line) or inhibition of protein synthesis [translational inhibition] (dashed line), the mass fraction of proteins devoted to the synthesis of new proteins is a linear function of the growth rate. The puzzle remains as to how the enormous collection of highly nonlinear chemical reactions occurring within the bacterium give rise to such strong *linear* relationships between these two important macroscopic variables.

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A model for the effect of chemotherapy on the hematopoietic system

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We present the use of a physiologically-based model to represent possible pharmaceutical interventions and relate them to physiological parameters. We introduce a structured model for the production and regulation of blood cells taking the form of a system of nonlinear delay differential equations. This model contains multiple time delays to incorporate maturation and lifespan times of the different cell species, together with feedback mechanisms controlling the rate of maturaions : some of the delays are therefore state-dependent. Concentrating on the regulation of neutrophils, we analyse equilibrium solutions and their destabilisation by Hopf and secondary bifurcations, giving a dynamical interpretation to neutropenic episodes and obtaining conditions for the simultaneous stability of multiple equilibria. This model is then used to represent the effect of current chemotherapeutic regimens (paclitaxel) on neutrophil levels, including the influence of scheduling, as well as the remedial use of G-CSF

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Non-invasive Dermal and Transdermal Delivery Systems for Macromolecules

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The delivery of drugs through the skin provides a convenient route of administration that is often preferred to injections because it is non-invasive and can usually be self-administered, improving patient compliance. Unfortunately, a major obstacle to both dermal and transdermal drug delivery is the resilient barrier that the epidermal layers of the skin provide against exogenous chemical agents. The advancement of transdermal drug delivery will require the development of novel delivery systems that are suitable for modern, macromolecular protein and nucleotide therapeutic agents. Significant effort has been devoted to obtain a functional understanding of the physical barrier properties imparted by the epidermis, specifically the membrane structures of the stratum corneum. However, structural observations of membrane systems are often hindered by low resolution, leading to difficulties when attempting to determine molecular mechanisms related to interactions between lipids found in the stratum corneum. Several models describing molecular diffusion of drug molecules through the stratum corneum have been postulated. Chemical permeation enhancement is thought to disrupt lipid organization, leading to an increase of membrane fluidity and consequently the rate of drug diffusion into the circulatory system. Recent investigations suggest an alternate mechanism could involve the formation of unique membrane phases, leading to the formation of aqueous channels through which macromolecules could freely diffuse. In this review, we discuss the advantages and limitations of permeation enhancing strategies and how computational simulations on the atomic scale, coupled with physical observations can provide insight into the mechanisms of diffusion through the stratum corneum.

AMMCS-2011

Minisymposium: Modeling in Biophysics

SS-MBP

Organizers:
Bae-Yeun Ha, *University of Waterloo (Canada)*
Mikko Karttunen, *University of Western Ontario (Canada)*

This minisymposium is to discuss recent advances in our quantitative understanding of biology. It will seek to identify challenges at the interface between the physical and biological sciences, and explore computational and soft matter approaches to solving them.

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Emergence of long time scales and stereotyped behaviors in C. elegans

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Animal behaviors are often decomposable into discrete, stereotyped elements, well-separated in time. In one model, such behaviors are triggered by specific commands; in the extreme case, the discreteness of behavior is traced to the discreteness of action potentials in the individual command neurons. Here, we use the crawling behavior of the nematode C. elegans to demonstrate the opposite view, in which discreteness, stereotypy and long timescales emerge from the collective dynamics of the behavior itself. In previous work, we found that as C. elegans crawls, its body moves through a "shape space" in which four dimensions capture 95% of the variance in body shape. Here we show that stochastic dynamics within this shape space predicts transitions between attractors corresponding to abrupt reversals in crawling direction. With no free parameters, our inferred stochastic dynamical system generates reversal time scales and stereotyped trajectories in close agreement with experimental observations. We use the stochastic dynamics to show that the noise amplitude decreases systematically with increasing time away from food, resulting in longer bouts of forward crawling and suggesting that worms can use noise to modify their locomotory behavior.

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Relationship between model bacterial peptidoglycan network structures and AFM force-distance curves

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Recent atomic force microscopy (AFM) measurements have involved pulling on Gram-negative bacterial sacculi with the AFM tip as a means of distinguishing between different proposed structures of the peptidoglycan network. The goal of the present study is to provide the theoretical connection between a given network structure and its response to the pulling force. We model the glycan strands as hinged rods, and the peptide cross-links as wormlike chains. Using Monte Carlo simulation to equilibrate the three-dimensional network, subject to a fixed AFM tip-to-substrate distance, we can compute the force exerted by the network on the AFM tip. The effects of adhesion of the sacculi to the substrate and enzymatic action on the network are included. We examine both the layered and the scaffold model for the peptidoglycan network structure. We comment on the differences in the response of these two models, and make comparisons with experiment.

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The Iceberg model of hydration and its breakdown: interplay of structure and dynamics in hydrophobic hydration

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The effect of temperature on the dynamics of hydration water around a hydrophobic molecule, tetramethylurea (TMU), is studied using ab initio Car-Parrinello Molecular Dynamics (CPMD). We conduct a systematic study spanning a wide temperature range (230 K–450 K) at low TMU concentration. Our study provides a unified and consolidating picture of hydration at the microscopic level, and resolves several outstanding issues: 1) We show the existence of 3 relevant times scales, their precise microscopic origin and importance. 2) We provide a full microscopic picture of the long debated "iceberg"; model [1], showing its limits, and how it breaks down at low temperatures. This resolves the controversies and unifies the picture provided by recent femtosecond-Infrared (fs-IR) [2], THz-GHz dielectric relaxation [3] and NMR experiments [4]. In particular, we show how solvation water rotates faster than bulk water at supercooled temperatures around T=250 K. 3) We confirm the liquid-liquid critical point hypothesis of supercooled water as proposed by Poole et al almost 20 years ago [5]. Finally, the radial distribution data suggests that hydration water forms strata within the solvation shell, thus indicating that the slowing down of solvation shell water may not be uniform through out the shell. Dynamics of water molecules is of central importance.

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Ring polymers in a confined space as model bacterial chromosomes

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Chromosomes in living cells are strongly confined and yet show a high level of spatial organization. Similarly, confined polymers display intriguing organizational and segregational properties. Here we discuss how ring topology influences self-avoiding polymers confined in a cylindrical space – it not only stiffens individual chains but also enhances their segregation, as if they were in a narrower cylinder. Our polymer model is used to analyze the long-standing observations of chromosome organization and segregation in *E. coli*.

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Hybrid continuum-MD approach to simulating mesoscopic systems

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Many biological systems are at an intermediate mesoscale- too big for a full molecular dynamics simulation yet too small and complex for a reliable simulation based on continuum modelling. I will describe a hybrid method that combines continuum fluctuating hydrodynamics [1] with molecular dynamics, allowing discrete objects of arbitrary shape and stiffness to interact with a background fluid. As an example I will discuss the use of a nanowire as a local probe of elasticity [2].

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Volumetric properties of the hydrophobic interaction: Pressure dependence

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Pressure experiments have become common tools to probe biomolecules along the reaction coordinate determined by the volume of the system. In agreement with Le Chatelier's principle, increasing pressure in proteins leads to unfolding as pressure-unfolded-configurations occupy smaller volumes compared to the native state. Being able to determine the microscopic mechanism related to pressure unfolding and in particular the interactions that give up first in this process is essential to understand protein stability and by extension the limits under which proteins can function. While the nature of the culprit interaction responsible for pressure unfolding is still under debate [1], strong evidence points to the hydrophobic interaction [2].

Here we use all atom simulations to explore volumetric changes upon non-polar hydration at different pressures. We focus on how the volume of the system depends on the distance between a pair of solutes at different pressures as opposed to previous studies on the hydration of single solute [3][4]. Understanding this dependence is important to account microscopically for pressure unfolding [2].

In addition to the volume, compressibility is also measured experimentally during pressure unfolding. In this paper, we present all atom-simulations for changes in compressibility during non-polar hydration. These results are used to rationalize models for pressure unfolding of proteins. Time permitting we will discuss the pressure versus temperature phase diagram of proteins with emphasis in the role played by the hydrophobic interaction. Cold denaturation will also be discussed [5].

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Adsorption of Inhibitor Peptides on Hydroxyapatite and Calcium Oxalate Monohydrate Surfaces: A Computational Study

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Protein-mineral interactions play a key role in the development of new diagnosis and treatment protocols for several major diseases, such as arterial calcification, osteoporosis and dental erosion [1][2][3]. Under physiological conditions the solvating medium typically contains peptides which are intimately involved in the mineral formation. Both nucleation and inhibition of crystal growth has been shown to be subject to significant modifications as a function of the biological regulatory protein concentration.

There are still substantial uncertainties in how these regulatory peptides interact with mineral surfaces. The physical and chemical mechanisms to control and direct the growth process are not yet understood in full microscopical detail. This is partly because the span of the relevant time scales is wide and partly because the constituent molecules are highly complex.

Molecular dynamics simulations have been shown to provide clues to the possible mechanisms of protein-regulated biomineralization. As a methodology molecular mechanics is a relatively new technique in the field. In this study we combine and compare computational and experimental studies side by side. We focus on hydroxayapatite (HA) and calcium oxalate monohydrate (COM) crystals, which both are medically and technologically important examples of the general problem.

We discuss how electrostatics plays an important role in the adsorption of peptides on the calcium rich surfaces[1]. We discuss how post-translational modifications affect the qualitative properties of the peptide-mineral binding[2][3]. We also study the dominant surface steps and kinks and correlate the computional results to experimental data.

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A Mathematical Model for Spherical Ionic Micelles In the Presence of Excess Salt

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We present a model to describe the aggregation size distribution of the spherical micelles of Sodium Hexa Sulfate (SHS) and Sodium Dodecyl Sulfate (SDS) in the presence of excess salt (sodium chloride) in the solution. The model is based on numerical solutions of a set of kinetic equations,

$$K^+_{1,2}C_1^2 + (\sum_{n=2}^{M-1} K^+_{n,n+1}C_n)C_1 - (\sum_{n=1}^{M-1} K^-_{n+1,n}C_{n+1}) = 0$$

$$(K^-_{n,n-1} + K^+_{n,n+1}C_1)C_n - K^+_{n-1,n}C_{n-1}C_1 - K^-_{n+1,n}C_{n+1} = 0, \quad n = 2,3,\ldots,M-1.$$

In above equation C_n is the concentration of micelles with n surfactants and M is the largest size of micelles in the system. Constant rates $K^+_{n,n+1}, K^-_{n+1,n}$ are respectably addition and removal rates. Our assumption was that the micellar aggregation is a stepwise process and also surfactant addition/removal rates are considered to depend on micelle size.
The constant addition rates are calculated from the Smoluchowski model which treats the process of cluster formation as a sequence of random collisions between free surfactant and cluster. Removal rates calculation based on the micelles Gibbs free energies. In calculating Gibbs free energies for each size of micelles for different concentration of added salt we used the molecular thermodynamics models by Nagarajan and Rucenstein [1]. This model for ionic free energy consider the approximate analytical solution to the Poisson-Boltzmann equation. The results were compared to the size distributions obtained from the Molecular Dynamics simulations of SHS [2] and SDS [3][4]. This model can predict the aggregation sizes of micelles and their dependence on excess salt concentration without considering the atomistic details.

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Minisymposium: Mathematical and Computational Modeling of Influenza

SS-MCMI

Organizers:
Catherine Beauchemin, *Ryerson University (Canada)*
Hana Dobrovolny, *Ryerson University (Canada)*

Applications can come from industry or from research in the sciences, for example, from applied and pure mathematics, the natural sciences, engineering and economy.Despite the ongoing threat of a severe influenza pandemic and extensive research on this topic,there is still much we do not understand about influenza. In this minisymposium, the speakers will cover various aspects of the disease for which mathematical and computational modelling can provide precious assistance in analyzing available data, extracting additional information, and predicting outcomes.

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The Impact of Vaccination During the 2009/2010 pH1N1 Epidemic in Montreal, Quebec, Canada

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The 2009/2010 pandemic of influenza H1N1 is studied using Montreal as the focal population. Data on confirmed cases and weekly vaccination rates are used to construct a mathematical model that can simulate the epidemic in Montreal. The epidemic is then simulated with the effect of the vaccination removed. The estimated number of cases, hospitalizations and deaths averted through the vaccination campaign are found. In total, approximately 921,000 vaccinations are associated with the prevention of between 90 and 436 hospitalizations averted and 4 and 19 deaths averted, depending on the assumed relationship between vaccination and onset of immunity. The results are of interest to public health officials for evaluating the impact of vaccination.

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A simulation platform to enhance pandemic preparedness and responses to future pandemics in Ontario

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Mathematical modelling has long been used in the study of infectious disease epidemiology, but the full utility of mathematical models for public health application has not yet been realized. In 2009, during the emergence of pandemic H1N1, mathematical modellers were given the opportunity to contribute to the decision-making process through working groups of mathematical modellers such as PanINFORM. However, decision makers had only six months after the emergence of the novel virus to prepare and to implement adequate mitigation strategies for Fall 2009; mathematical modellers had even less time to develop suitable models in order to provide advice to them. Models specific to pandemic H1N1 had to be developed from scratch. Moreover, the questions that needed answering were continually evolving as new information came to the fore. Such events highlighted the need to have a suite of pre-existing, generic models that can be taken off the shelf and efficiently adapted to a new pathogen. We are presenting a highly functional, multi-level social network simulation model used as a platform for modelling transmission and control of an epidemic within a population of a mid-size city. The platform consists of two components: (1) a population generator that represents the demography and social structure of a population as a social network, and (2) a suite of disease transmission modules that represents how a novel pathogen spreads through this network and how it is controlled. The social network created by the population generator consists of interacting agents whose activities are based on pre-observed rules of social interactions, independent of emerging pathogens. The disease transmission modules are then separately created to mimic the spread of a particular disease. Unlike in traditional mathematical models, where the model design and its implementation follow a linear process creating a model with limited upgrading abilities, the proposed model design is based on a functional independency. This approach has numerous advantages, the most significant of which is providing the model with the ability to incorporate the new information and hence to timely upgrade. This characteristic of the model design considerably reduces the amount of time required to develop models to inform disease control and mitigation strategies, and thus expand the utility of such models enormously.

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The impact of individual and social psychology on the effectiveness of vaccination against infectious diseases

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Ring vaccination has been found to be an effective and affordable strategy to eliminate certain infections. For instance, ring vaccination was credited in the final stages of smallpox eradication. Ring vaccination attempts to reach all contacts of an initial index case, and vaccinate them vaccinate to control the spread of the disease. There has been little research on mathematical modeling of ring vaccination where the contacts of the index case choose whether or not to vaccinate based on criteria such as payoff functions. Our model considers an index case with N susceptible contacts who have a tendency to vaccinate or not based on their payoff to vaccinate versus payoff not to vaccinate. The individuals' decision is based on this tendency, but may also be influenced by imitating the tendencies of other individuals within the ring. With the introduction of imitation, we found that the probability of containing the disease outbreak through ring vaccination changes considerably. Under imitation processes and when stochastic heterogeneity is present, very different outcomes from different stochastic realizations using the same parameter distributions are possible, ranging from complete containment to complete non-containment. This occurs even when the equivalent solution of rational behaviour (no imitation) contains mixed strategies. Imitation thus magnifies the choice of either vaccination or non-vaccination, so in some realizations the choice of the majority is vaccination and reducing the number of secondary infections, while in other realizations based on the same parameter distribution, the majority chooses not to vaccinate. Therefore, the effectiveness of ring vaccination can strongly depend on the imitation process, and imitation can introduce a level of uncertainty as to how effective ring vaccination will be. We conclude that risk communication efforts should be initiated early in an outbreak, and this is especially true within communities where peer opinion is a strong force in vaccinating behaviour. Under the condition that ring vaccination fails and an infection becomes established in a population, the question naturally arises as to how individual vaccinating behaviour responds to endemic infection. This requires considering transmission across the entire social network, not just in the contacts of an initial index case. Hence, in the second part of the talk we will discuss the transmission of an influenza type infection through a network. Individuals tend to base future decisions on their own past history of infection. If an individual has to make the choice of whether or not they want to vaccinate for the upcoming season they take their infection history into account, as well as perceived vaccination risks, since perceived risk/cost depends on past experiences. Our model considers how an individual's past experiences, over a given number of years impacts the payoff functions and their decision, and how this changes according to network type. We will present preliminary results using return maps to characterize coupled behaviour-incidence dynamics over multiple seasons, highlight the kinds of surprising results that can emerge in models that capture feedback between individual immunizing behaviour and population-level disease incidence levels. The combination of transmission across networks and human behavioural responses has the potential to improving our understanding of infectious disease transmission, as well as controlling the disease, in situations where individual behaviour matters. This is joint work with Chris Bauch.

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Mechanistic modelling of the three mortality waves in the 1918 influenza pandemic in the UK

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Multiple waves have been observed in the initial phase of influenza pandemics, notably the 1918 pandemic. The mechanisms that account for this phenomenon remain unclear. Here, we show that we can fit the three mortality waves observed in the 1918 pandemic in the UK using a simple compartmental disease model which allows transmission rate to be affected by school terms, weather, and behavioral responses to mortality. Using a likelihood-based inference method, we found that all three factors are needed to reproduce the observed pattern. In particular, behavioral response to mortality is required for a model to display three waves.

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Effects of Environmental Conditions on the Dynamics of Avian Influenza among Wild Birds

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The emergence of the highly pathogenic avian influenza (AI) sub-type H5N1 in many parts of the world has focused greater attention on the ecology of influenza in wild birds, as wild birds are the major natural reservoir for all known influenza A viruses. The persistence of avian influenza viruses in water, which is highly affected by environmental conditions, plays an important role in AI transmission in wild birds. We will present mathematical models that include bird migration as well as the experimentally-derived relationships between viral persistence and environmental conditions. We first demonstrate that the model is consistent with field survey data from Northern Europe, and predict the effects of temperature, pH and salinity on the basic reproductive number (R0). Our results show that environmental variations strongly affect both single season and long-term AI dynamics. In addition, environmental variations predict several interesting features of AI dynamics which are observed in real data: peak-time variation, place-to-place variation and seasonal double peaks (summer and fall).

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Analysis of a spatial model for influenza viral infections

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Influenza A virus infection of the respiratory epithelium triggers an antiviral innate immune response. This takes the form of secretion of type-1 interferons from infected epithelial cells and release of inflammatory and chemotactic cytokines from alveolar macrophages, and from mobile neutrophils and dendritic cells following phagocytosis of virus particles produced by infected epithelial cells. This activates natural killer (NK) cells and produces viral antigen-bearing macrophages and dendritic cells, leading to clonal expansion of influenza-specific cytotoxic T lymphocytes (CTLs). Activated NK cells can kill newly-infected epithelial cells whereas anti-influenza CTLs destroy virus-producing epithelial cells.

The objective of this work is to establish the threshold conditions under which a viral infection of the respiratory epithelium can be overcome by the innate immune response. Knowing the threshold, or even determining qualitatively how to avoid it (i.e., ensure that infection does not spread), is of direct clinical importance in avoiding severe infections, and a problem well-suited to modelling. This is an extension of earlier work Ref. [1] showing the importance of the killing rate of infected cells (particularly by CTLs) in containing the spread of an infection. We formulate a spatial model for the influenza virus infection, including spreading infection of epithelial cells by delayed virus replication Ref. [2], and interactions with mobile activated NK cells and CTLs. Critical conditions are established for the onset and spread of infection in the respiratory tract. By modelling the spatially-smoothed kinetics of these processes, it is possible to gain insights into critical mechanisms implicit in the control of virus infection. We analyze the model to investigate the role of the immune response in preventing events such as the generation of an unwanted “cytokine storm" and ensuing inflammation in the respiratory tract.

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Full viral kinetic parameterization of a pair of seasonal H1N1 influenza virus strains in vitro: An application to antiviral resistance

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The 2008–2009 influenza season saw a dramatic increase in cases of antiviral drug-resistance. In that season, prior to the emergence of the swine-origin pandemic influenza (pH1N1), nearly 100% of H1N1 viruses isolated from patients were found to have the H275Y mutation of the neuraminidase gene which confers resistance to oseltamivir (Tamiflu), up from 10% in the previous year and less than 1% in prior years [1]. Although antiviral resistance has currently declined again, due to the dominance of the oseltamivir-susceptible pH1N1, the sudden and spontaneous development of resistance to the primary anti-influenza drug was both troubling and unexpected. In fact, it had long been thought that the H275Y mutation was a crippling mutation which so impaired a virus' replication ability that it would be unable to compete with wild-type (susceptible) strains (see, e.g., [2]). In this situation, it is imperative to understand the fundamental viral kinetic properties which have allowed for the dominance of an oseltamivir-resistant strain.

Here, we have performed a set of classical in vitro experiments (including plaque and viral yield assays [3]) on a pair of seasonal influenza strains — one susceptible and one resistant to oseltamivir — and applied a family of mathematical models to the time-series data in order to extract the full set of kinetic parameters controlling the virus-cell interaction for each strain. To our knowledge, this is the first complete specification of an influenza virus infection in vitro. The techniques we have introduced will allow for the rapid characterization of new virus strains in the future and may be useful in identifying the specific phases of the influenza virus replication cycle which are interrupted by new and existing antiviral drugs.

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The effect of virion external packaging on the dynamics of drug-resistant influenza virus

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Influenza virus has a high mutation rate which can lead to the rapid development of drug resistant strains. Models used to study the emergence of drug resistance typically assume that the mutant strain always carries the surface proteins, and thus the drug susceptibility, of the mutant virus. However, this may not necessarily be the case for a drug-resistant mutant produced within a cell infected by wild-type virus. When a cell is infected, it expresses viral surface proteins on its own membrane. The cell membrane is then borrowed by the virus to produce an envelope for the virion. Thus when a wild-type strain infects a cell wild-type surface proteins will appear on the cell membrane. If a mutation conferring drug resistance occurs in that cell, the envelope of the resulting drug resistant virion will retain the wild-type surface proteins.

We investigate the effect of viral external packaging on the emergence of drug resistant mutants in influenza virus through the use of mathematical models. We propose several variations of a two virus model, assuming either that mutant virus produced within a wild-type cell retain the wild-type drug susceptibility or that they have the drug susceptibility of the mutant strain. Through computer simulation, we determine what effect the mutant virion external packaging has on the emergence of drug resistance. We find that when mutant virions intially retain the surface proteins of the wild-type strain the number of breakthough infections is reduced and the mutant virus becomes detectable later in the infection. Our models indicate that virion external packaging is an important factor in the emergence of drug resistant influenza strains.

AMMCS-2011

Mathematical Modeling in Neuro-science

SS-MMNS

Organizers:
Shoja Chenouri, *University of Waterloo (Canada)*
Paul Marriott, *University of Waterloo (Canada)*

The increase in quality and quantity of data in modern neuroscience presents many new challenges for mathematical modelling. The session looks at a range of approaches to this area; mathematical, statistical and computational. It aims to give a general mathematical audience a sense of what is happening in the exciting new area.

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Prediction and connectivity in fMRI studies of stroke recovery

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Functional neuroimaging studies have two main goals: the clinical goal of making predictions that are useful in diagnosis and treatment, and the scientific goal of understanding which areas of the brain do what and how they interact. We have addressed both types of question in our analysis of two longitudinal functional magnetic resonance imaging (fMRI) studies of recovery from stroke: one concerning strokes that affect the motor area [1][2], and one ongoing study concerning aphasia caused by stroke.

Towards the goal of clinical prediction, we compared ten methods of binary classification of fMRI images, including: linear and quadratic discriminant (on an optimised number of principal components); support vector machines with linear, quadratic and radial basis function (RBF) kernels; and two novel methods based on pairs of restricted Boltzmann machines (RBM), which are stochastic recurrent neural network models. On the motor stroke data we found that, while performance varies considerably across subjects and classification tasks, the best overall performers were nonlinear: quadratic discriminant, support vector machines with RBF kernels, and generatively-trained pairs of RBMs. I will also discuss ongoing work on generative models of images and image sequences, and their use in prediction.

We also studied aspects of *functional connectivity*, i.e. correlations between the activities of different brain areas. We considered measures of complexity of connectivity, including an estimated rank of the signal covariance in a probabilistic PCA (principal component analysis) model, which in the motor stroke study, had a positive correlation with a measure of degree of recovery. Further, we identified brain regions involved in changes in connectivity during recovery from motor stroke, including the cerebellum and the motor area contralateral to the lesion.

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Applying optimal hierarchical controllers to neural models of motor control

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Optimal control theory and hierarchical structures have long been thought integral to biological motor control systems, and evidence supporting these ideas continues to grow. The application of these techniques to neural systems models, however, is unclear. Our research focuses on bridging the gap between control theoretic and neuroscientific models of motor control.

Here, we present work building on research from [DeWolf, 2010] and [DeWolf, 2011], where the Neural Optimal Control Hierarchy (NOCH) framework was presented, which maps mathematical characterizations of the control problem onto neural systems. Specifically, we show how optimal feedback control in a hierarchical system governed by a component-based linear Bellman controller [Todorov, 2009] operating on a high-level abstracted representation of the system can be mapped to specific neural sub-systems. We employ this system to demonstrate that optimal feedback control theory, compositionality of movements, and hierarchical control structures can be combined in a biologically constrained fashion to reproduce normal human arm trajectories and velocity profiles. Further, we demonstrate that impairing various components of the model associated with specific neural systems can account for the motor deficiencies seen in patients with analogous damage. Specifically, we demonstrate this behaviourally for both Huntington's disease and cerebellar damage [Smith, 2000]. In addition, we show how this same model can be implemented at the level of individual spiking neurons. This low-level model provides a novel account of pre-movement and movement spiking neural activity recorded from the motor cortex of monkeys [Churchland, 2010].

We suggest that these results provide support for the NOCH framework, and that this approach can be used to provide both more biologically-relevant constraints on optimal control models as well as new insights and experimental directions for biological investigations of the motor system.

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Computational Graph Theoretical Model of the Zebrafish Sensorimotor Pathway

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Mapping out the detailed connectivity patterns ('connectomes') of neural circuits is a central goal of neuroscience and has been the focus of extensive current research [1][2]. The best quantitative approach to analyze the acquired data is still unclear but graph theory has been used with success [2][3]. We present a graph theoretical model of such a connectome, with vertices and edges representing neurons and synaptic connections, respectively. Our system is the zebrafish posterior lateral line sensorimotor pathway. In fish, lateral line hair cells on the skin surface are stimulated by water currents, triggering neural activity that propagates first to ascending sensory neurons, then to processing circuits in the brain, and finally to spinal cord circuits that encode the motor response to the stimulus. This system is biologically well-studied and includes many 'identifiable neurons' whose position and connectivity pattern is persistent across essentially all individuals. The goal of our analysis is to elucidate mechanisms of information processing in this neural pathway by comparing the mathematical properties of its connectome graph to those of other, previously described graphs. We create two biologically plausible models based on currently known anatomical data. The two models differ primarily in their connection patterns from the brain to the spine. In the first, every descending (brain) neuron is assumed to have the same total number of connections. In the second, each descending neuron sends the same number of connections to every spinal segment it connects to, thus, descending neurons connecting to a larger number of segments are assigned more connections. The degree distributions and small-world measures of the two realistic models are compared to small-world, random and structured random graphs of the same size (with over 2500 nodes and 160,000 connections). For each type of graph, 100 randomly generated instantiations are considered. Comparisons of the two realistic models further includes vulnerability to random edge deletion and deletion of neurons (Mauthner cell and its homologues) established to be important in the zebrafish startle response. We find that both of the anatomically-based graphs show small-worldness similar to other neural networks, but do not have a scale-free distribution of connections. Ongoing studies are examining the effects of lesioning the Mauther cell and its homologues to determine if the model will reproduce known behavioral effects of such lesions. This study is a novel approach to the computational analysis of the zebrafish nervous system. Our results suggest specific hypotheses for future biological studies of this neural pathway and for computational investigations on the role of connection density and connection patterns in a neural network.

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EEG Source Modeling with Variational Bayes

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An EEG recording is a measure of the electric field potential at the scalp due to primary current sources within the brain. These recordings have greater temporal resolution than other brain imaging techniques, but do not provide a clear picture of the spatial properties of the signal. A key problem in EEG analysis is source reconstruction, the problem of estimating the primary current distribution within the brain from scalp recordings.

The source reconstruction problem is under determined, there are an infinite number of source configurations which will result in the same scalp distribution. This problem is also made difficult from the presence of noise in the signal. This noise can be due to other biological signals such as muscle activity or external influence such as recording equipment. The problem of source reconstruction is thus somehow a question of selecting the 'best' solution based on some criteria.

One option is to impose restrictions to the solution based on physiology, for example requiring a smooth solution or constraining the sources to be oriented perpendicularly. Another option is to parametrize the solution as a small number of discrete currents and then estimate their location and orientation, such a method is motivated mathematically more than biologically.

A Bayesian framework has been developed for model selection in such complex problems. This framework is ideal for the source reconstruction problem because it allows the researcher to guide the solution with their prior information. One problem with this framework is that it is often not possible to calculate the posterior distribution analytically. The classical way to deal this problem is to use MCMC methods to generate a random sample from the posterior distribution. There is tremendous computational burden in performing sampling based algorithms for realistic sized models, thus there is a need for more efficient algorithms that are still able to capture the important details of the solution.

Recently a method known as Variational Bayes has been used to approximate the posterior distribution. The Variational Bayes approximation assumes independence between groups of parameters. In many cases under this assumption, the form of the approximating distribution can be identified, then its parameters can be fit to maximize the evidence for the model.

Using a hierarchical linear regression model to describe EEG recordings, the two methods of calculating the posterior distribution are compared. This is a simulation study using basic but realistic head models.

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Multiscale, multivariate spike train analysis

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This research proposal introduces a new methodology for the analysis of neural spike trains. Mathematical/statistical models are powerful tools in modeling biological aspects of interest. The biological properties, and how they are reflected in neural data, are introduced in this research proposal. Some of these biological aspects motivate multiscale frameworks, which allow for simultaneous modeling of the local and the global behavior of neurons. A detailed literature review of the applications of such models is provided. It is also shown, through some case studies, that the multiscale penalized likelihood method is a powerful model in explaining many of these biological points of interest. To detect periodic activities of neu- rons, a periodicity detection test is adjusted for the multiscale penalized likelihood model. The challenging problem of multivariate analysis of the neural spike trains is also addressed. As far as we know, the multivariate models which are available in current literature suffer from limited dependency structures. To address this issue, the Skellam process, as well as the multivariate Skellam random variable, which have flexible dependency structures, are developed. A computationally efficient recursive algorithm for the estimation of the parameters is also introduced. A plan of future work for the thesis is provided.

AMMCS-2011

Mathematical Modeling of Protein Flexibility

SS-MMPF

Organizers:
Forbes Burkowski, *University of Waterloo (Canada)*
Henry Wolkowicz, *University of Waterloo (Canada)*

In biology, modeling the structure of a large molecule is very important if one is to understand its behaviour. Structure models have been utilized in the analysis of DNA, RNA, and proteins. In particular, proteins have a very complicated structure that allows them to interact with each other and with smaller molecules. The "magic" that is life takes place in the cavities of their macromolecular surfaces. A protein is a long chain-like molecule, typically involving thousands of atoms, and usually folded into a compact low energy structure. Living cells contain tens of thousands of different proteins that provide both structure and control of life processes. To understand these processes we need to study both the 3D structures of proteins and the structural changes that are intrinsic to protein functionality. This session of the conference will deal with the geometric modeling and computational algorithms related to these structural changes.

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Predicting protein hinge motions and allostery using rigidity theory

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Given the 3-D structure of a protein (i.e. PDB file), understanding how it functions depends in critical ways on predicting which parts are rigid, and which are flexible. We can model the molecule like an engineered structure of fixed units (atoms with their bond angles as rigid units, bonds as potential hinges) plus biochemical constraints coming from the geometry (hydrogen bonds, hydrophobic interactions). This generates a 'molecular graph' in the theory of combinatorial rigidity. Drawing on graph theoretic algorithmic methods for bar-body frameworks (the $6|V|-6$ pebble game), as well as the recently solved 30 year old molecular conjecture, a basic algorithm on the molecular graph makes flexibility/rigidity predictions for the molecular structure [4][5]. The pebble game algorithm is embedded in an online FIRST server for fast predictions of flexible and rigid regions in a protein [1][3].

In our recent work we have extended the pebble game algorithm to specify regions that are relevant as constraints with respect to a specified region and those that are irrelevant [4]. In this study we further extend this basic model and the algorithms and offer a novel hinge prediction algorithm. Hinge motions occur between two rigid domains and are essential for a large repertoire of biological functions, and comprise the largest class of known protein motions as depicted in the Database of Macromolecular Motions (MOLMOV) [2]. We have tested our hinge prediction algorithm on several proteins, chosen from the dataset of manually annotated hinges publicly available on the MOLMOV site. Many of our predictions are in very good agreement with this data set. Our algorithms can also be used to give predictions of 'allosteric' interactions in proteins- where binding on one site of a molecule changes the shape or binding at a distance 'active site' of the molecule.

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On the Universal rigidity of bar frameworks in general position

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A bar framework $G(p)$ in$r$-dimensional Euclidean space is a graph G whose vertices are points $p^1,..,p^n$ in R^r, and whose edges are line segments connecting pairs of these points. A given framework $G(p)$ in R^r is said to be universally rigid if there does not exist a non-congruent framework $G(q)$ in any Euclidean space with the same edge lengths as those of $G(p)$. A framework $G(p)$ in R^r is generic if the coordinates of$p^1,..p^n$ are algebraicaly independent over the integers. On the other hand, $G(p)$ is in general position in R^r if there is no subset, of cardinality $r+1$, of the points$p^1,..,p^n$ that is affinely dependent.

It is known that a generic framework $G(p)$ on n vertices in R^r is universally rigid if and only if $G(p)$ admits a positive semi-definite stress matrix of rank $n-r-1$. In this talk, I'll show that the "if" part of this result still holds under the weaker assumption of a framework in general position. It is still unknown whether or not the "only if" part of the above result holds under the general position. However, it is shown that it holds if graph G is the $(r+1)$-lateration graphs.

Universal rigidity has many important applications in molecular conformation and wireless sensor networks.

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LoopWeaver - Loop Modeling by the Weighted Scaling of a Verified Protein

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When one is creating a theoretical model of a protein using using threading techniques, or creating an actual model based on NMR data, there will be regions with no prediction available, called gaps. These regions are typically highly variable coil regions, and this high variability makes perfect template matches unlikely. The high flexibility of these coil regions also makes them difficult, or impossible, to determine by NMR. These regions can play an important role in how the protein interacts, so accurate loop modeling (the modeling of a short loop of protein to fit into a gap) is very important to understanding the roles proteins play in biology.

We introduce a new method for fitting existing loops, obtained from a database of known protein structures, into these gaps While existing database solutions accomplish the same goal, it is difficult to fit many existing loops while keeping realistic dihedral angles at the edges of the gap, avoiding clashes with the rest of the protein chain, and maintaining the shape of the database loop. Our program, LoopWeaver, uses multidimensional scaling (as described in [1]) in order to both fit database loops with minimal changes to the loop, and adjust those loops to avoid clashing with the existing proteins.

As with other database methods, LoopWeaver works very well when combined with an ab-initio technique. For example, on our test set of 60 loops of length 10, selected from CASP8 and 9 targets, the Loopy[2] program achieves an average local RMSD (all backbone atoms) of 1.9 angstrom. By using the DFire energy potential[3] to pick from either Loopy or LoopWeaver results, this can be improved to an average of 1.6 angstrom. While other database methods can make improvements to ab-initio techniques, our results are more significant. Additionally, many of these other database techniques are unable to fit appropriate matches to a substantial portion of loops to be modeled. This is acceptable when taking consensus between several methods, as a missing result only means you must rely on other techniques for that specific loop. Because of the multidimensional scaling step, to improve the fit and avoid clashes, we have been able to fit loops into every gap tried so far, even very large gaps. The average local RMSD of our results, on the CASP8 and 9 targets, is very similar to that of Loopy (1.9 for the length 10 target set), with no targets being skipped due to a lack of non-clashing matches.

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Protein flexibility of dimers: Do symmetric motions play a role in allosteric interactions?

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It is well-understood that the functioning of a protein depends on have basic stable forms (tertiary structure) and having some residual flexibility supported by that structure. The modeling of protein flexibility and rigidity in terms imported from physics and engineering has been developed within the theory of rigid frameworks and is available via fast combinatorial algorithms in programs such as FIRST: flexweb.asu.edu), and is described in papers such as [2][3]:

Recent work in rigidity theory has modified this analysis and the algorithms to account for basic symmetry of the structure and motions which preserve this symmetry. In particular, a framework which would normally count to be combinatorially minimally rigid in generic realizations has been shown to become flexible when realized with 2-fold rotational symmetry in 3-space [3].

Protein dimers, formed by two copies of a protein are a good case study for the possible impact of this added flexibilty, as they generally self-assemble with 2-fold rotational axis, for reasons of minimal energy [1]. What is the significance the behaviour dimers, such as tryptophan repressor? There are several possibilities: (i) the pathway of a symmetry preserving motion may better support the allostery, so that when one tryptophan binds (or leaves) the entire protein is pushed along to make the same change at the second binding site; (ii) while the dimer may not be flexible, without breaking some hydrogen bonds, the initial breaking and binding at one site may be pushed back toward symmetry, so that the symmetric bonds break and the second binding is afforded.

We will explore this case study and consider other possible ways to integrate symmetry information into the analysis, including other symmetries which are found in proteins. We will also discuss further areas of work.

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AMMCS-2011

Mathematical Models in Social Sciences

SS-MMSS

Organizer:
Marc Kilgour, *Wilfrid Laurier University (Canada)*

The Social Sciences offer broad ranges of problems, issues, and principles that can benefit from mathematical modelling. In fact, many of the Social Sciences have taken an increasingly mathematical flavour over the last 75 years, and a great deal of interesting mathematics has resulted from this cross-disciplinary collaboration. For example, Game Theory, which was developed by a renowned mathematician, John von Neumann, and a well known economist, Oskar Morgenstern, has revolutionized Economics, and made substantial impacts in Political Science and other disciplines. This session will feature a new applications of mathematics and mathematical models to problems in the social sciences, and includes new ideas for bargaining, social choice, psychology, and other fields.

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Quasiutilitarian social choice with approximate interpersonal comparison of welfare gains

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Let $\mathscr{X}$ be the set of all possible psychophysical states which any human being could be in at a moment in time. We assume that an element of $\mathscr{X}$ encodes all ethically relevant information about the physical and mental state of a person. Suppose it is possible to make approximate interpersonal comparisons of welfare gains and losses. Thus, if $w,x,y,z \in \mathscr{X}$, then it is sometimes possible to say, "The welfare gain of the state change $w \mapsto x$ is greater than the welfare gain of the state change $y \mapsto z$." We can represent this by the formula "$(w \mapsto x) \succeq (y \mapsto z)$", where $(\succeq)$ is a *differential preorder*: an incomplete preorder on the space $\mathscr{X} \times \mathscr{X}$ of all possible personal state changes.

Let $\mathscr{I}$ be a finite or infinite set, representing a set of people. A *social state* is an element $\mathbf{x}$ in the Cartesian power $\mathscr{X}^{\mathscr{I}}$, which assigns a psychophyiscal state x_i in $\mathscr{X}$ to each i in $\mathscr{I}$. A *social state change* $(\mathbf{x} \mapsto \mathbf{y})$ can thus be seen as a bundle $(x_i \mapsto y_i)_{i \in \mathscr{I}}$ of personal state changes. A *social differential preorder* (SDP) is an incomplete preorder on the space $\mathscr{X}^{\mathscr{I}} \times \mathscr{X}^{\mathscr{I}}$ of social state changes, which satisfies two properties: *Anonymity* (i.e. invariance under finite permutation of coordinates) and *Pareto* (with respect to the differential preorder on personal state changes). We will define and characterize several SDPs.

The *minimal* SDP is the natural extension of the Suppes-Sen preorder to this setting; we show it is a subrelation of every other SDP. The *approximate utilitarian* SDP ranks social state changes by comparing the sum total utility gain they induce, with respect to all 'utility functions' compatible with $(\succeq)$. The *net gain* preorder ranks social state changes by comparing the aggregate welfare gain they induce upon various subpopulations. We show that, under certain conditions, all three of these preorders coincide. We apply this theory to a model of redistributive wealth transfers. This shows that it is possible to develop a nontrivial social choice theory, even with a very limited and approximate structure of interpersonal welfare comparisons.

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Narrowing the Field in Elections: The Next-Two Rule

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We suggest a new approach to narrowing the field in elections, based on the deservingness of candidates to be contenders in a runoff, or to be declared one of several winners. Instead of specifying some minimum percentage (e.g., 50) that the leading candidate must surpass to avoid a runoff (usually between the top two candidates), we propose that the number of contenders depend on the distribution of votes among candidates. Divisor methods of apportionment proposed by Jefferson and Webster, among others, provide measures of deservingness, but they can prescribe a runoff even if one candidate receives more than 50 percent of the vote. We propose a new measure of deservingness, called the Next-Two rule, which compares the performance of candidates to the two that immediately follow them. It never prescribes a runoff when one candidate receives more than 50 percent of the vote. More generally, it identifies as contenders candidates who are bunched together near the top and, unlike the Jefferson and Webster methods, never declares that all candidates are contenders. We apply the Next-Two rule to several empirical examples, including one (elections to major league baseball's Hall of Fame) in which more than one candidate can be elected.

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A Procedure for Fair Division of Indivisible, Identical Objects with Entitlements

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Allocating objects fairly in a way that provides the maximum satisfaction to all individuals involved is not always a trivial task. Fair division procedures are developed to address this issue. A problem of fair division of indivisible, identical objects with different entitlements arose in the study of the satisfaction approval voting system (Brams and Kilgour, 2010). This voting system can be used in a proportional representation context to translate parties' levels of support into an allocation of the available seats. This allocation is defined as the one that maximizes the total satisfaction of all voters. The satisfaction of a voter is given as the proportion of his or her preferred candidates who are elected. The electorate is partitioned into supporters of the various parties; each party knows this division, and can assume that its own supporters will vote for exactly its candidates. Hence, the number of supporters a party has translates to a party's entitlement to the available seats. The fair division problem arises as the parties decide how many candidates to run.

To state the problem more generally, this paper uses terms such as players, objects and entitlements rather than parties, seats and supporters respectively. The problem is modeled using game theory, as the players must decide how many objects to demand. After a discussion of the Nash Equilibria of the games, a rounding rule is given based on the number of available objects and each player's entitlement. From this rounding rule, players can determine how many objects to demand and how many they should expect to receive.

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A Simple Bargaining Mechanism That Elicits Truthful Reservation Prices

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We describe a simple 2-stage mechanism that induces two bargainers to be truthful in reporting their reservation prices in a 1st stage. If these prices criss-cross, the referee reports that they overlap, and the bargainers proceed to make offers in a 2nd stage. The average of the 2nd-stage offers becomes the settlement if both offers fall into the overlap interval; if only one offer falls into this interval, it is the settlement, but is implemented with probability $\frac{1}{2}$; if neither offer falls into the interval, there is no settlement. Thus, if the bargainers reach the 2nd stage, they know their reservation prices overlap even if they fail to reach a settlement, possibly motivating them to try again.

The description of the new mechanism will be augmented with a comparison to the theoretically-best Chatterjee-Samuelson mechanism. As well, it will be compared to other mechanisms that induce honest revelation of reservation prices, using probabilistic implementation or externally-funded bonuses.

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Game Theory and Social Psychology: Conformity Games

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A game model is defined for situations involving social biases and conformity pressures that lead to potentially unfavourable behaviour in social groups. A simple model is described first, followed by a more complex model which takes into account the psychological biases false uniqueness and false consensus. The second model predicts a phenomenon studied in social psychology called pluralistic ignorance, which arises as a result of the prevalence of false uniqueness and the desire to conform. An efficient method is developed for finding Nash equilibria under certain restrictions.

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Generalizations and asymptotical results for stochastic rumour models

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Daley-Kendall and Maki-Thompson models are the two most cited stochastic models for the spread of rumours phenomena, in scientific literature. In both, a closed homogeneously mixing population is subdivided into three classes of individuals called ignorants, spreaders and stiflers, [1][4]. After a rumor is introduced in the population, it spreads by following certain rules that depend on the class to which the individual who knows the rumor belongs. The final proportion of the population never hearing the rumor is a variable of interest for the proposed models.

We establish asymptotical results for general stochastic rumour processes that have as particular cases the classical Daley-Kendall and Maki-Thompson models, and other variations for rumour models reported in the literature recently, [2][3].

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Serving Strategy in Tennis: Accuracy vs. Power

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Serves are a key part of the game of tennis, and are well-known to confer a significant advantage on the server. A crucial aspect of this advantage is the opportunity allowed a server who has faulted (delivered an out-of-bounds serve) to repeat the serve—once—thereby creating a unique two-trials scenario. Common practice is to hit a powerful and/or "tricky"; first serve, which has a high probability of faulting but, if in-bounds, a high probability of winning the point. If there is a fault, the second serve tends to be much weaker, and therefore less risky but easier to return. Recently it has been argued that this strategy is flawed, and that the second serve should be as powerful or as tricky as the first. We characterize serving strategies by the probabilities that the serve will land in-bounds and the probability that it will be returned successfully. Then we find optimal levels of risk for both serves, utilizing the contingent plans for the second serve in selecting the strategy for the first. We show that, optimally, the second serve should be less likely to fault than the first. In an effort to measure this probability gap, we extend our model to include the rally that would occur if a serve were successfully returned and show how optimal serve characteristics depend on the parameters of the rally. Based on examples, we make some inferences about the size of the probability gap.

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Mathematical Models for Nanoscience and Nanotechnology

SS-MNANO

Organizers:
Zoran Miskovic, *University of Waterloo (Canada)*
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Nanoscience may be defined as confluence of natural sciences, each contributing its traditional concepts and methods towards applications in Nanotechnology. Mathematical modeling in this interdisciplinary context has become a broadly based and exciting endeavor that helps understand phenomena at the nanoscale. This session aims at providing examples of mathematical models with contemporary applications in Nanoscience and Nanotechnology.

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Correlations in superconducting nano-wires

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The physical properties of superconductors at nano-scales differs from the bulk. Lower critical temperature or in some cases even the absence of the superconducting phase and residual resistivity in the superconducting phase are few properties that change when we reduce the size to nano-scales. In order to account for these effects a model has been introduced by Zaikin, Golubev based on the effective action method. In this talk, we will look at the correlations in this theory that are used in calculating transport properties of superconducting nano-wires. More specifically we will look at ac-conductivity in superconducting nano-wires.

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Theoretical Modeling of the Donor-Acceptor Pair Photoluminescence Dynamics in Ga_2O_3 Nanocrystals

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Transparent conducting oxides (TCOs), such as ZnO, SnO_2, In_2O_3 and Ga_2O_3, have drawn considerable interest among researchers over the years due to their polymorphic crystal structures, transparency and electrical conductivity. Among TCOs Ga_2O_3 has exceptionally wide band gap (4.9 eV), while retaining high electrical conductivity and featuring strong blue photoluminescence (PL). This combination of properties, arising from the presence of native defects, makes Ga2O3 exceptionally interesting for integrated opto-electronic applications. In particular, oxygen vacancies in Ga_2O_3 play a significant role in the blue emission, through the donor acceptor pair (DAP) recombination mechanism. The mechanism of the observed emission can be understood in a two step process. The first step is the formation of trapped excitons through the transfer of an electron in the donor states to the neutral acceptor. In the second step the blue emission is created through radiative recombination of the exciton on the acceptor sites.

We have recently developed a method for the synthesis colloidal γ-Ga_2O_3 nanocrystals, and demonstrated their size-tunable photoluminescence energy and decay rate [1]. In this talk we will present our recent progress in theoretical modeling of this size dependent PL decay in the framework of the DAP model [2]. The original DAP model was developed for random distribution of donors over large volume of bulk material in the presence of a small concentration of acceptors [2]. We have adapted the original DAP model for nanocrystals and developed two different models based on the location of donors and acceptors. In three dimensional (3-D) model, we assume a single acceptor in the center of a sphere surrounded by randomly distributed donors, as majority defects. In the two dimensional (2-D) model, the donors and the acceptor are distributed across the surface of the nanocrystals. This study suggests that our experimental PL decay dynamics data are best fit to the 2-D model for nanocrystals of different diameters. The importance of these results for optimizing and manipulating defect-based PL in nanostructured materials, and understanding the defect formation in NCs will be discussed.

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Ionic Screening of Charged Impurities in Graphene

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Besides recent interest in applications of carbon nano-structures for nano-electronic devices, these structures also show great promise in applications for chemical and biological sensors. While carbon nanotubes have been extensively studied in that context, reports on using graphene as biochemical sensor are only beginning to appear. Graphene operates in such applications in the configuration of a field-effect transistor with its surface exposed to an electrolyte containing mobile ions. By applying a gate potential through the electrolyte, one may achieve a control of graphene's conductivity that is extremely sensitive to the presence of adsorbed molecules, ion concentration, or the pH in an aqueous solution. In that context, we have recently developed a model of electrolytically top-gated graphene, taking into account nonlinear polarization of graphene [1], as well as the ion crowding effect in the nearby electrolyte due to different ion sizes [2].

Particularly intriguing is dual-gated graphene, where the presence of charged impurities in the oxide layer underneath graphene affects its conductivity [3]. It was shown experimentally that the ions in the electrolyte above graphene provide efficient screening of the charged impurities, thereby improving conducting properties of graphene by increasing the mobility of its charge carriers [4]. We study this problem by means of the partially linearized Poisson-Boltzmann theory that was used for the liquid-solid interfaces containing random distribution of charges [5]. We first evaluate the screened potential in the plane of graphene due to a single point-charge impurity in a substrate such as SiO_2. Further, we assume a random distribution of charged impurities in the substrate and evaluate the autocorrelation function for the screened potential in graphene. By using this result in a self-consistent theory of graphene transport based on the Boltzmann kinetic theory [3], we show that the mobility of charge carriers in graphene increases with increasing salt concentration in the electrolyte, in accordance with the experimental observation [4].

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Hybrid Continuum and Molecular Modeling of Nano-flows

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A novel hybrid method combining the continuum approach based boundary singularity method (BSM) and the molecular approach based direct simulation Monte Carlo (DSMC) is developed and then used to study viscous fibrous filtration flows in the transition flow regime. First, the flow about a single fiber confined between two parallel walls is used to test the proposed hybrid method. The DSMC is applied to an annular region enclosing the cylinder and the BSM is employed to the entire flow domain. The parameters used in the DSMC and the coupling procedure, such as the number of simulated particles, the cell size and the size of the coupling zone are determined by inspecting the pressure drop obtained. It is observed that in the partial-slip flow regime the results obtained by the hybrid BSM-DSMC method match the ones from the BSM combined with the heuristic partial-slip boundary conditions. For higher Knudsen numbers, the difference in pressure drop and velocity is significant. The developed hybrid method is then parallelized by using MPI and extended for multi-fiber filtration flows. The multi-fiber filter flows considered are in the partial-slip and transition regimes. For , the difference in pressure drop between the BSM and hybrid method appears to be less than 10%. For , the difference in pressure drop approaches 20%. The computed velocity near fibers changes even more significantly with the increase of the Knudsen number, which confirms the need of molecular methods in numerical evaluation of the flow in filters. Applications of the proposed numerical methodology include multi-particle interactions in constructing nano-structures by self-assembly, the nano-scale fluid motion in synthesis of carbon nanotubes by chemical vapor deposition process, particle capture mechanisms in filtration, signaling and sensing, to name a few applications. The proposed combined continuum and molecular methodology can incorporate surface chemical reactions and the electromagnetic forces in the DSMC procedure for Knudsen layer.

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Mathematical Modeling of Single Semiconductor Quantum Dots

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Single quantum dots (QD) exhibiting an intrinsic excitonic fine structure are being the most promising nanostructures for the aim of single and polarization-entangled photon generation [1]. Particularly, creating deterministic sources of entangled photons has recently become an intriguing subject in this context.

In this work, we mathematically model the optical characteristics of a typical semiconductor quantum dot. We first calculate the single particle wavefunctions along with their corresponding discrete energy levels through strain-dependent *k.p* envelope function approximation [2]. The governing hamiltonian is essentially the modified version of Kane's model for zinc-blende III-V materials including strain-induced coupling between conduction and valence subbands in addition to spin-orbit interaction.

Moreover, realistic modeling of the QD emission behaviour comprises the excitonic nature of the system, which in turn, demands for finding the few particle states and their transition oscillator strengths. Consequently, we employed Configuration Interaction (CI) method to account for the spin character of multiexcitons localized inside the QD: CI approach incorporates many-body correlation effect by constructing the excitonic states through a linear combination of a given orthogonal set, here provided by *k.p* method as the underlying band structure [3].

We also demonstrate how built-in piezoelectric potential associated with the off-diagonal components of the strain tensor may reduce the lateral symmetry of the QD envelope functions giving rise to long range exchange interactions, and hence, trivial bright state splitting. This energy separation between exciton bright states is the origin of entanglement demolition in deformed or asymmetric QDs.

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Nonequilibrium Dynamics of a Superconducting Plasmonic Channel

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We present a mathematical model to identify dynamical properties of a weak-coupling BCS superconductor irradiated by an optical source where the number of superconducting pairs greatly exceed the number of quasiparticle (QP).

The model employs a combination of coupled phonon-quasiparticle rate equations [1] with Parker's time-dependent T^* model [2] to determine nonequilibrium properties such as effective electron temperature, diffusion length scale and energy gap. This energy gap is then used to drive an expression for the transient complex conductivity [3]. The resulted relation predicts a sudden increase of loss at the gap frequency ($E = 2\Delta$) and a high frequency behavior similar to normal metals in terms of optical conductivity. Considering this dispersive nature, we demonstrate the possibility of using this class of materials as a negative index layer to excite surface plasmon polariton waves when it is embedded in an infinite homogeneous dielectric media [4].

Furthermore, to characterize the system, the dispersion of the electromagnetic modes and power propagation lengths as a function of film thickness and width is calculated when a p-polarized volume electromagnetic wave propagates toward the channel.

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Numerical Analysis of Parametric and Nonlinear Wave Interaction in Discrete Josephson Transmission Line

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A novel superconducting Transmission Line (TL) which is periodically loaded by Josephson junctions (JJ) is proposed as a platform to realize a traveling-wave parametric amplifier. Using TL model, this structure is modeled by a system of nonlinear partial differential equations (PDE) with a driving source and mixed-boundary condition at the input and output terminals, respectively. This model successfully emulates parametric and nonlinear microwave propagation when long-wave approximation is applicable.

A rigorous and robust Finite Difference Time Domain (FDTD) solver based on the explicit Lax-Wendroff and implicit Crank-Nicolson schemes has been developed to investigate the device responses under various excitations [2]. Linearizing the wave equation, under small-amplitude assumption, dispersion and impedance analysis are performed to explore more aspects of the device for the purpose of efficient design of a traveling-wave parametric amplifier.

Knowing all microwave characteristics and identifying different regimes of operation, which include impedance properties, cut-off propagation, dispersive behavior and shock-wave formation [1], we exploit perturbation theory accompanying with the method of multiple scale to derive the three nonlinear coupled amplitude equations to describe the parametric interaction. A graphical technique is suggested to find three waves on the dispersion diagram satisfying the phase-matching conditions. The incorporation of two numerical techniques, spectral method in space and multistep Adams-Bashforth in time domain, is employed to monitor the unilateral gain, superior stability and bandwidth of this structure.

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AMMCS-2011

Minisymposium: Numerical Methods for Mathematical Models Based on ODEs, PDEs, Integral and Integro-differential Equations

SS-NMMM

Organizers:
Atife Caglar, *University of Wisconsin - Green Bay (USA)*
Faranak Pahlevani, *Penn State University, Abington College (USA)*

This minisymposium covers all aspects of numerical methods for mathematical models based on ODEs, PDEs, integral and integro-differential equations. Numerical methods play a fundamental role in mathematical modelling. Mathematical models comprise the development and study such as structure, well posedness, and solution properties of a mathematical formulation of a problem. Numerical methods comprise the formulation and study such as stability, convergence, computational complexity of a numerical approximation or solution approaches to a mathematically formulated problem. Applications may be drawn from the broad range of physical, life, social sciences, as well as from many engineering and industrial disciplines.

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Analysis of long time stability and errors of two stable partitioned methods for uncoupling evolutionary groundwater-surfacewater flows

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This report analyzes and tests two partitioned methods that require only one, uncoupled Stokes and Darcy sub-physics and sub-domain solve per time step for the fully evolutionary Stokes-Darcy problem. From considering the exactly skew symmetric coupling of the two problems, we derive two, special purpose partitioned methods. Under a modest time step restriction of the form $\triangle t \leq C$ where $C = C(physical\ parameters)$ we prove unconditional asymptotic (over $0 \leq t < \infty$) stability of the partitioned method. From this we derive an optimal error estimate that is uniform in time over $0 \leq t < \infty$.

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Perturbation methods for vibrations of moderately elliptical plates

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The governing equation of a vibrating thin plate is given by biharmonic equation $\nabla^4 W - k^4 W = 0$ where $k^2 = \omega r^2 \sqrt{\rho h/D}$, ω is the natural frequency, ρ is the density, D is the flexural rigidity, h is the thickness, and r is the some length scale (radius of the averaging circle). The fundamental frequency, which is the smallest eigenvalue of the equation corresponding to the unidirectional mode with no nodal diameter, plays a crucial role when designing plates in applied sciences, since the resonance is not possible when the plate is excited by a frequency lower than the fundamental frequency.

Fundamental frequencies of vibrating plates have been determined only for a limited class of plate geometries. Vibration of circular plates were first studied by Lord Raleigh [1]. An extensive survey of plates is given in a monograph by Leissa [2]. While circular and rectangular plates have been extensively studied, in the case of elliptic plates, very few result appear in the literature. Most of the literature on the subject are concentrating in numerical methods especially for full elliptical plates. However, in some cases especially when numerical methods become inadequate, such as plates with small internal supports, numerical methods often encounter the problem of singularity, scaling, and sensitivity to the boundary conditions.

In this work with C.Y. Wang [3], we investigate vibrations of moderately elliptic plates using a boundary perturbation method developed by [4][5]. It was shown in [4][5] that the problems in circularly periodic domains can be treated by solving sequence of biharmonic eigenvalue problems for which corresponding perturbed boundary conditions are prescribed. The method is used to extract the fundamental frequencies of moderately elliptic plates with and without core support. Outer boundary conditions used in this work is clamped and simply supported. Inner boundary condition for the core is clamped, simply supported, and free. In the absence of a core, frequency comparisons with other authors are in agreement. The technique yields an analytic approximate formulations to the fundamental frequencies of such plates, using the boundary perturbation method in the case of clamped and simply supported outer boundary conditions.

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Superconvergent Collocation Interpolants for Delay Volterra Integro-Differential Equations

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Collocation methods generating continuous polynomial approximations to DVIDEs involve solving implicit system of equations over each step of integration. The size of the implicit system grows proportional to the desired off-mesh point accuracy. For 'non-standard' Volterra integro-differential equations with constant delay that often arise in modeling predator-prey systems in Ecology, the collocation solution is C^0 continuous and is less accurate than the discrete approximation. The accuracy is $O(h^{s+1})$ at off-mesh points and $O(h^{2s})$ at mesh points where s is the number of Gauss points used per subinterval and h refers to the stepsize. We will show how to construct C^1 interpolants using a few extra **explicit** computations (without increasing the size of the implicit system) so that the accuracy at off-mesh points and mesh points is of the same order. This implies that even for coarse mesh selections we can achieve an accurate and smooth approximate solution. Specific schemes are presented for $s = 2, 3$, and numerical results demonstrate the effectiveness of the new interpolants.

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Parameter Sensitivity of Eddy Viscosity Models with Applications

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Large Eddy Simulation (LES) is a technique for simulation of the turbulent flow using a filtering procedure on Navier-Stocks equations, ultimately solving the equation for the average velocities. Averaging the Navier-Stocks equations affects the reliability of the solution. Therefore assessing the uncertainty of the applied LES model is an important issue. Sensitivity analysis is one current mathematical approach to investigate this problem. [1][2]

In this presentation, sensitivity analysis of the Eddy Viscosity Models (EVM) from the class of LES models with respect to the variation of eddy viscosity parameter is discussed. The application of the sensitivity computations in improving flow functionals and identifying the reliable values of the parameter of interest is illustrated by two experiments: flow around a cylinder and the driven cavity problem. [1][3]

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Cell-Centred Finite Difference Methodology for Solving Partial Differential Equations on an Unstructured Mesh

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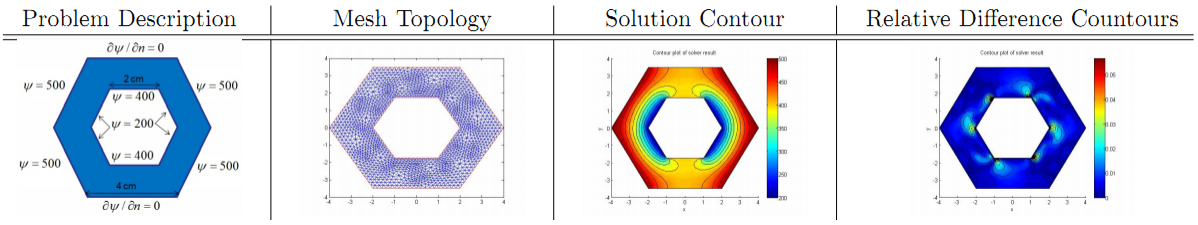
A new cell-centred finite difference (CCFD) numerical methodology for structured, unstructured or hybrid mesh topologies is proposed. The methodology is designed to solve a variety of partial differential equations (PDEs) governing physical phenomena, such as electrostatic potential in electromagnetic fields, solid and fluid mechanics, heat transfer and wave phenomena. In the CCFD numerical scheme, central finite differencing is implemented at cell centroids by taking differencing points along orthogonal Cartesian axes localized within each cell. Differencing points in each cell are expressed in terms of cell centroid and nodal values by weighted average or element interpolation function approximations, as used in the finite element method. Once all cell centroid values are determined, interior and Neumann boundary nodes can be approximated by weighted average of neighbouring cell centroid values. As such, a linear system is developed with $N+M$ equations, where N is the number of interior and Neumann nodes and M represents the number of cells in the mesh. The equations of this system are linearly independent in $N+M$ dimensional space and so a unique solution exists. The system of equations can be solved by either direct or iterative approaches.

The new CCFD methodology is applied to several "benchmark" physical problems, covering typical model equations such as elliptic, parabolic and hyperbolic PDEs along with boundary and initial conditions. The numerical solution of these "benchmark" problems will be compared to exact analytical solutions if available, or results from other types of numerical simulations, such as finite element and finite volume methods.

To illustrate the method, consider a steady heat transfer problem in a 2D hexagonal ring. The temperature distribution is governed by an elliptic PDE, $\div(k\,T)=0$. The boundary is subjected to constant Dirichlet and zero-flux Neumann conditions. This problem is solved on a triangular mesh with 1536 nodes and 2880 cells, using both finite element and the CCFD method. The mean relative difference over the entire physical domain, calculated as $\frac{1}{N}\sum_{i=1,\psi_{e,i}\neq 0}^{N}\left|\frac{\psi_{e,i}-\psi_i}{\psi_{e,i}}\right|$, is about 0.70% with highest error clustered at the discontinuity boundary corners. The advantages of the proposed new scheme and directions for further research will also be discussed.



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Nested Uzawa algorithms in models for the cementing of oil and gas wells

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Primary cementing of oil and gas wells is a common operation during well construction, in which drilling mud is displaced with a cement slurry. The displacement flow can be modelled in laminar regime using a Hele-Shaw modelling strategy, reducing the problem to an elliptic variational inequality coupled to an advection equation. The variational inequality arises due to the fact that drilling muds and cement slurries may have a yield stress. In recent years the industry has moved towards horizontal well drilling, and for these wells it is common to move the casing during cementing. Although physically beneficial, mathematically this increases the problem complexity considerably. The Hele-Shaw approach leads to a closure problem for the local fluid flow (on the gap scale) that must itself be solved iteratively, before the displacement flow can be computed. We outline the algorithm we have used for this - a nested series of Uzawa algorithms each solving an augmented Lagrangian saddle point problem. Sample results are presented.

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A Finite Element Approximation of Navier-Stokes Alpha Model

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In this talk, we present a finite element formulation of NS-Alpha model under non- periodic boundry condition. We give semi and full discretization of the model and provide error estimates.

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Numerical study of the slip with friction boundary conditions for the regularized Navier-Stokes equations

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The computational challenge of fluid flow simulation lies in dealing with the tremendous range of spatial eddy scales. Direct numerical simulation (DNS) approaches for the Navier-Stokes equations (NSE), without averaging any of the structures/eddies, presents a formidable computational challenge for accurate simulation at high Reynolds numbers. For this reason, regularization models of the NSE have been studied during the years, resolving motions only above some critical scales. These models allow for accurate and efficient simulations of high Reynolds-number flows, while resolving only large-scale flow structures/eddies, for which it is natural to apply slip with friction boundary conditions, [1]. Theoretical and numerical investigations for slip with friction boundary conditions applied to the Navier-Stokes equations (NSE) and other fluid models have been done, see [2] and its references.

We study the effect of the slip with friction on the boundary where vortices are generated coupled with time relaxation regularization of the Navier-Stokes equations. The aim of the regularization term is to drive the unresolved fluctuations in a simulation to zero exponentially fast by an appropriate and often problem dependent choice of its coefficient, [3]. The family of models is coupled with slip with friction boundary conditions, discretized with finite element method, and second order Crank-Nicolson temporal discretization. The obtained numerical algorithm is tested on the 2D benchmark step problem. The numerical experiments show a successful shedding of the eddies behind the step, which is the essential feature of the step flow problem.

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AMMCS-2011

Physics and Mathematics of the Human Placenta

SS-PMHP

Organizers:
Dimitri Vvedensky, *Imperial College London (UK)*
Carolyn Salafia, *Placental Analytics LLC (USA)*

This special session will discuss the development of models and techniques, both theoretical and experimental, in the fields related to the human placenta. One of the examples includes models for the morphological evolution and vascular structure of the human placenta.

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The Placenta: The Mathematics of Life Before Birth

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Understanding risk factors for disease is key to their early diagnosis and possible cure. In the last decade, it has been increasingly appreciated that complications of pregnancy carry risk of increased maternal morbidity and mortality, but also are associated with increased lifelong health risks for the newborn infant, child and adult. This has been termed "fetal programming". The health risks are not only broad (many diseases associated with pregnancy complications) but also robust, having been demonstrated in both genders, in developing and developed countries and as early as the teen years. Many studies have used birth weight, the summation of both genetic influences on size from the parents and the nutrition provided by the placenta, as a proxy for intrauterine "wellbeing"; greater or lesser birth weight, all other factors being equal varies lifelong health risks. Genetics aside, the principal determiner of birth weight is the placenta, the organ responsible for transport of all nutrients that compose the newborn. Pathologists measure organs like the placenta in daily practice, with rulers, and semiquantitative scores of features seen on light microscopy. Evidence suggests that placental structure is intimately tied to its function, and that that structure is, at some level, fractal. The insights gained by applying mathematics and physics to this organ have improved our understanding of the timing, and present clear testable hypotheses regarding the causes of intrauterine stressors that may be responsible for fetal programming. Improved neonatal risk assessment for disorders as diverse as obesity and autism may allow early intervention and optimize outcomes for the child, the family and society.

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Translating Innovative Mathematical and Physical Measures of the Placenta into Predictors of Childhood Health: The Journey from Mathematics and Physics to Pathology to Epidemiology

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Our multidisciplinary team draws on the disciplines of mathematics, physics, pathology, and epidemiology in studying the role of the placenta as a predictor of later health outcomes. Our work has collectively demonstrated that more nuanced and quantified measures of shape and structure of the placenta, derived from principles of mathematical and physical modeling, can predict a range of childhood outcomes. Future work will focus on quantification of vascular branching patterns of the placental surface as early predictors of autism. In this talk, I will "translate" the measures of the placenta as developed by the team and review our findings to date that link these measures to later health outcomes. Potential mechanisms for the associations between the placenta and health outcomes will also be discussed. We will present data published from the Collaborative Perinatal Project, a study with poor placental measures that nonetheless show significant effects of different placental shapes and thickness on age 7 year body mass index, diastolic blood pressure and IQ. For the former we hypothesize that different shaped placentas are composed of different proportion of nutritive villi, and villi that provide part of the total peripheral resistance of the child's, and those differences are what account for the body habitus and blood pressure changes. In regards to IQ, we found no correlation of IQ with disk thickness when disk thickness was at least average (2 cm), but a significant negative association with thinner placentas. We hypothesize here that branching growth of the placental vasculature is controlled by the same gene families and signals that control neuronal branching growth and in this case, the reduced disk thickness that means reduced placental vascular branching is a direct mirror of reduced neuronal branching in the fetus. We currently have an Innovative Idea Award in Autism research to explore this further.

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Why is there variety in placental shape: early influences vs trophotropism?

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Several years ago we proposed a qualitative model of growth of placental vasculature based on a stochastic growth process known as Diffusion Limited Aggregation (DLA) The model has allowed us to view the placental shape at delivery as a record of a dynamical process of growth affected by maternal stressors, genetic pre-disposition, and by random factors. Our modeling suggests that not only the most common abnormalities of placental shape but also non-centrality of umbilical cord insertion result from early influences. In contrast, the current conventional wisdom explains such abnormalities as a result of trophotropism: the placenta grows where it can, and does not grow where it cannot. We use the data of ultrasound studies of placentas in the first trimester, which recorded the three-dimensional shapes of the placentas at 11-14 weeks and at delivery at term, to see which explanation is better. Our findings validate our empiric modeling. Early influences are largely responsible for marginality of the umbilical cord insertion (and resulting lowered placental functional efficiency). Bi-lobate placental shape reflects a deformation of the early vasculogenic zone. The evidence suggests that the early growth of the placenta is typically not round, but follows the few main branches of the vascular tree; if the secondary branches of the vascular tree grow normally, then this shape rounds out later in gestation. Perturbation of vascular growth no later than the mid trimester that precluded or limited would account for regularly-irregular shapes at term.

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Combining Multiple Cues for Automated Histopathology Image Analysis

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The presence and number of inflammatory polymorphonuclear leukocytes ("neutrophils") is a useful indicator of inflammation in placental tissue. In the previous work by Thomas, Sottile, and Salafia, an automatic method was developed to identify the neutrophils in digitized slide images. While the method is based on valid principles, its performance is limited due to the biological variety in real images. In this work, we improve the method of Thomas et al. for vascular smooth muscle by incorporating multiple detection cues under a fuzzy logic framework. Particularly, we develop two additional cues: (1) to distinguish normal tissue nuclei from neutrophils, we test that the apparent neutrophil is not surrounded by tissue, (2) since neutrophils tend to form clusters, we identify nuclei with high cluster density. We show that these cues are combined naturally with the fuzzy logic framework and that the combination improves detection and outperforms any one cue used individually.

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Perceptual normalized information distance for image distortion analysis based on Kolmogorov complexity

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Image distortion analysis is a fundamental issue in many image processing problems, including compression, restoration, recognition, classification, and retrieval. Traditional image distortion evaluation approaches tend to be heuristic and are often limited to specific application environment. In this work, we investigate the problem of image distortion measurement based on the theory of Kolmogorov complexity, which has rarely been studied in the context of image processing.

This work is motivated by the normalized information distance (NID) measure that has been shown to be a valid and universal distance metric applicable to similarity measurement of any two objects [1]. Similar to Kolmogorov complexity, NID is non-computable. A useful practical solution is to approximate it using normalized compression distance (NCD) [1], which has led to impressive results in many applications such as construction of phylogeny trees using DNA sequences [1]. In our earlier work, we showed that direct use of NCD on image processing problems is difficult and proposed a normalized conditional compression distance (NCCD) measure [2], which has significantly wider applicability than existing image similarity/distortion measures.

To assess the distortions between two images, we first transform them into the wavelet transform domain. Assuming stationarity and good decorrelation of wavelet coefficients beyond local regions and across wavelet subbands, the Kolmogorov complexity may be approximated using Shannon entropy [3]. Inspired by [4], we adopt a Gaussian scale mixture (GSM) model for neighboring wavelet coefficients and a Gaussian channel model for the noise distortions in the human visual system. Combining these assumptions with the NID framework, we derive a novel perceptual normalized information distance measure, where maximal likelihood estimation and least square regression are employed for parameter fitting. We validate the proposed distortion measure using three large-scale, publicly-available, and subject-rated image databases, which include a wide range of practical image distortion types and levels. Our results demonstrate the good prediction power of the proposed method for perceptual image distortions.

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Statistical Topology of the Human Placenta

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The vascular system of a placenta has a branching structure within the chorion that resembles a tree. The origin of the tree is the umbilical cord insertion in the placenta. The vasculature and its branching points are represented by edges and vertices, respectively. An edge connects an nth generation vertex to an (n+1)th generation vertex. Two edges are sides of a triangle if its corners are a nth generation vertex and two (n+1)th generation vertices.This is the basis for representing the vasculature of a placenta as a structural triangulation. We describe a method for studying the properties of such radial networks based on the distribution of their energy states, as represented by this structural triangulation of the network. The partition function obtained from these states is used to calculate thermodynamic functions. The entropy, in particular, measures the distribution of triangulated areas in the tree. A high area distribution relates to a higher symmetry in the branching structure. By varying the distribution parameter, which is the inverse temperature in the statistical thermodynamic interpretation, one is able to weight generations of the network differently. This analysis identifies similar networks at their maturation state the state when the system stops growing as well as enabling the development of a network to be investigated. The latter feature is especially important for the placenta, where the details of the expansion of the network are typically not available. We provide several examples of such analyses for human placentas to illustrate the utility of our method and its potential in a clinical setting.

AMMCS-2011

Mathematical Modeling for Supply Chain and Product Development in High-Tech Industries

SS-SCPD

Organizer:
Amy H. I. Lee, *Chung Hua University (Taiwan)*

The manufacturing industry is undergoing a major transition to services, not just in sales but also in business structure. The move toward more extensive, customer oriented products and services has become common in many manufacturing industries, especially those that produce high-tech products. Thus, new product development and effective supply chain management are essential to obtain competitive advantages in todays global economy. Due to the complexity of the business environment, well-constructed models are necessary to facilitate relevant decision making. This special session aims to study the mathematical modeling for supply chain management and product development in high-tech industries.

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An Integrated Model for Supplier Selection for a High-Tech Manufacturer

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Global competitiveness has become the biggest concern of manufacturing companies, especially in high-tech industries. Improving competitive edges in an environment with rapidly changing technological innovations and dynamic customer needs is essential for a firm to survive and to acquire a decent profit. Thus, the introduction of successful new products is a source of new sales and profits and is a necessity in the intense competitive international market. A firm, in order to maintain its competitive edge, must protect its core businesses; however, it must be and usually is willing to enter buyer-supplier relationships due to limited resources. Therefore, after products are developed, the firm needs to cooperate with upstream suppliers to provide satisfactory components and parts for manufacturing final products. To achieve the benefits of buyer-supplier integration, in terms of increased internal efficiency and profitability of both parties, identifying and selecting viable suppliers is a preliminary step that needs to be properly managed.

Supplier selection works based on mathematical or quantitative decision-making approaches are increasing in the past decade. Mathematical programming (MP) models on supplier selection problem can be subdivided into linear programming, mixed integer programming, and goal programming/multi-objective goal programming (MOP). In recent years, many works of supplier selection have adopted analytic hierarchy process (AHP) or analytic network process (ANP), two famous multi-criteria decision making methodologies. Even though the research on supplier selection is abundant, the works usually only consider the critical success factors in the buyer-supplier relationship and do not emphasize the new product development (NPD) capabilities of the suppliers. The negative aspects of the buyer-supplier relationship and suppliers' NPD capabilities must be considered simultaneously in today's competitive high-tech industries. Thus, the objective of this paper is to propose an analytical approach to select critical-part suppliers under a fuzzy environment.

In this study, a comprehensive approach is proposed to select the most appropriate critical-part suppliers in order to maintain a high reliability of the supply chain. A fuzzy analytic network process (FANP) model, which incorporates the benefits, opportunities, costs and risks (BOCR) concept and considers the interrelationship among the factors, is constructed to evaluate various aspects of suppliers. A committee of experts in the industry is formed to define the supplier selection problem, and the problem is decomposed into a control hierarchy and a BOCR network. The control hierarchy is used to calculate the relative importance of benefits, opportunities, costs and risks merits. The BOCR network contains multiple factors that are positively or negatively affecting the success of the relationship. By taking into account experts' opinions and applying fuzzy set theory to consider information impreciseness, FANP is used to calculate the importance of the factors in evaluating suppliers. A performance ranking of the suppliers can then be obtained. The proposed model is adopted in a TFT-LCD manufacturer in Taiwan in evaluating the expected performance of suppliers with respect to each important factor, and an overall ranking of the suppliers can be generated as a result.

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New Product Development for Green and Low-Carbon Products – A Case Study of a TFT-LCD Manufacturer

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Green supply chain has become an important topic these days due to pollution, global warming, extreme climatic events, etc. From the Kyoto Protocol in 1997 to the United Nations Climate Change Conference (COP15) in Copenhagen in 2009, various countries are in agreement that environmental protection is essential and that reducing carbon dioxide (CO_2) emissions is the most important way to combat the climate change. In a conventional supply chain, cost, on-time delivery and quality are treated as the most important factors. However, such a rationale is out-dated and cannot keep a firm competitive in the market because of the increasing demands of green products. A green product is manufactured with the goal of reducing the damage to the environment and limiting the use of energy and other resources at any stage of its life, including raw materials, manufacture, use, and disposal. Carbon footprint is a good measure of the impact that a product has on the environment, especially in climate change, in the entire lifetime of the product. Carbon footprint is directly linked to CO_2 emission. Thus, the reduction of CO_2 emission must be considered in the product life cycle. Although more and more researchers are working on the green supply chain management in the past few years, few have incorporated CO_2 emission or carbon footprint into the green supply chain system. Therefore, this research aims to propose an integrated model for facilitating the new product development (NPD) for green and low-carbon products.

In the digital era, flat panel displays (FPD) is quickly becoming the preferred choice in many applications of human machine interface. With their low weight, slender profile, low power consumption, high resolution, high brightness and low radiance advantages, FPDs has been widely adopted from portable appliances to notebook and desktop monitors and even to large screen digital televisions. Thin film transistor-liquid crystal display (TFT-LCD), the primary FPD technology, occupies the majority of the FPD market, and Taiwan's production in TFT-LCD is one of the highest in the world. Even though the TFT-LCD industry is flourishing, it is becoming extremely competitive day by day. In this research, a systematic model based on quality function deployment (QFD) is constructed for developing green and low-carbon products in a TFT-LCD manufacturer. Literature review and interviews with experts are done first to collect potential customer attributes (CAs) and engineering characteristics (ECs) for developing and manufacturing green and low-carbon TFT-LCDs. Because of limited resources, the firm can only consider limited number of factors. Therefore, fuzzy Delphi method (FDM) is applied to extract the important CAs and ECs. Fuzzy interpretive structural modeling (FISM) is used subsequently to determine the interdependence among CAs, the interdependence among ECs, and relationship of CAs and ECs. A house of quality (HOQ) for product planning is built based on the results of the FISM, and pairwise comparison questionnaire is used to collect the opinions of the experts. Finally, fuzzy analytic network process (FANP) is applied to calculate the priorities of the ECs. The results shall provide important information for the TFT-LCD firm in designing a new green and low-carbon product. The model can also be tailored and applied by a manufacturer in developing products.

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Pickup and Delivery Problem with Stochastic Travel Times for Semiconductor Supply Chains

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As a semiconductor supply becomes widespread and the competition pressure is very fierce, the cross-company supply chain operations are even more complicated such that a semiconductor manufacturer needs to integrate and manage distribution in supply chain networks effectively and efficiently to increase their competition edge and profitability. In semiconductor factories, highly capacity utilization and efficiently production scheduling are essential due to the intensive capital investment. Under such circumstances, requests fail to arrive within time window may result in capacity idle and even deferral delivery. However, in practical vehicle routing, there will be uncertainty derives from the ambient trip-to-trip variation in travel times. Therefore, taking the stochastic travel times and time windows into account is of great importance when planning vehicle routes and schedules. In the fleet, to protect products from vibration during transportations, some vehicles are with special facilities dedicated for 8" wafers, some are dedicated for 12" wafers, whereas others are open for all types of products. When assigning requests to vehicles, the product/vehicle compatibility must be considered.

Chance constrained programming is defined as follows: Select certain variables as functions of random variables with known distributions in such a manner to optimize a functional of both classes of random variables subject to constraints on these variables which must be maintained at prescribed levels of probability (Charnes and Cooper, 1959; Charnes and Cooper, 1963). The chance constrained programming is its general form as:

Optimize $f(c,x)$

Subject to $P(Ax \leq b) \geq \alpha$ (1)

where A, b, c are not necessarily constant but have, in general, some or all of their elements as random variables. P is the probability measure of the given probability space of uncertain parameter and the vector α contains a prescribed set of constants that are probability measures of the extent to which constraint violations are admitted (Charnes and Cooper, 1963; Mitra, *et al.*, 2008).

This study investigates the practical pickup and delivery problem with stochastic travel times for semiconductor supply chains (SPDPSSC). In addition to the classical pickup-and-delivery constraints on pairing, precedence, and capacity constraints, the SPDPSSC also involves constraints on stochastic travel times, time windows, and product/vehicle compatibility constraints. Since several fundamental properties of deterministic pickup and delivery problems no longer hold when travel times are stochastic, the solution methodologies of SPDPSSC are more intricate. In this study, we describe the SPDPSSC in detail and formulate a chance constrained programming model to find a set of routes for the vehicles in order to accomplish a set of requests at minimum total travel distances under two kinds of chance constraints, time windows and driver duration, hold with a prescribed probability. By the implementation of the proposed model, the vehicle routing problem in semiconductor supply chain can be more integrated and applicable for the real-world applications.

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Multi-objective Programming for Lot-sizing with Quantity Discount

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Inventory management has always been a popular topic, and inventory models typically can be categorized into two groups: deterministic and stochastic. In deterministic models, all input data are assumed to be deterministic, and a mathematical programming model is usually sufficient to obtain the optimal solution. On the other hand, stochastic models are often limited to highly restricted assumptions, and the majority of current literature is a variation of the deterministic lot sizing problem. The most common stochastic lot sizing considers demand as the uncertain parameter. In addition, quantity discounts is an important issue in inventory management. The unit purchase price from a supplier is reduced when a large order is placed and a quantity offer discount is present. There are usually two major types of quantity discounts: all-units discount and incremental discount. Under the all-units discount, if the quantity purchased belongs to a specified quantity level predetermined by the supplier, the discounted price is applied to all units beginning with the first unit. There are often a few price breaks, and the unit discounted price decreases as the quantity level increases. Under the incremental discount, the discounted price is only applied to those units inside the price break quantity. Thus, different prices are applied to the units belonging to different price breaks.

The multi-objective programming (MOP) problem can be transformed into a mixed integer programming (MIP) model to solve the multi-period inventory problem and to determine an appropriate replenishment policy for each period. The objective is to minimize the total cost, which includes the ordering cost, purchase cost, shortage cost and holding cost in a planning horizon.

$$\text{Minimize } TC = \sum_{t=1}^{T} \Big[\sum_{i=1}^{I} o_i \times F_{it} + \sum_{i=1}^{I} P(Q_{it}) \times Q_{it} \times F_{it} + s \times L(z_t) \times \sigma_t^{+h\times(X_{t+1}+L(z_t)\times\sigma_t)} \quad (1)$$

where TC is the total cost; o_i is the ordering cost per replenishment from supplier i; F_{it} is a binary variable, equal to 1 if a purchase is made from supplier i in period t, and 0 if no purchase is made; $P(Q_{it})$ is the purchase cost for one unit based on the discount schedule of supplier i with order quantity Q_{it} in period t; Q_{it} is the purchase quantity from supplier i in period t; s is the shortage cost, per unit per period; $L(z_t)$ is the standardized number of units short of ending inventory level in period t; σ_t is the pool standard deviation of demand in period t; h is the inventory holding cost, per unit per period; and X_{t+1} is the expected beginning inventory level in period $t+1$.

Multi-objective programming (MOP) is one of the popular methods for decision making in a complex environment. In a MOP, decision makers try to optimize two or more objectives simultaneously under various constraints. A complete optimal solution seldom exists, and a Pareto-optimal solution is usually used. Some methods, such as the weighting method which assigns priorities to the objectives and sets aspiration levels for the objectives, are used to derive a compromise solution. The ε-constraint method is a modified weight method. One of the objective functions is optimized while the other objective functions are treated as constraints and are incorporated in the constraint part of the model. This research considers a stochastic lot-sizing problem with multi-suppliers and quantity discounts. The model is transformed into a mixed integer programming (MIP) model next based on the ε-constraint method. An illustrative example is used to illustrate the practicality of the proposed model. The results demonstrate that the model is an effective and accurate tool for determining the replenishment of a manufacturer from multiple suppliers for multi-periods.

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Maintenance Scheduling in Restructured Power Systems Using Benders Decomposition

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Maintenance outages of generating units should be scheduled and managed in an appropriate way such that the power demands are satisfied with high reliability and the minimum maintenance cost is obtained for power producers. This could be a very difficult and complex problem when the system contains multiple players including Independent Systems Operators (ISO) and Generation Companies (Gencos).

This is noticeable that all maintenance outages in restructured power system are generally supervised using ISO as a controlling and scheduling operator. Moreover, maintenance scheduling is a long-term horizon decision-making process in which the releases of generation units are constrained under predefined maintenance intervals. These intervals are obtained through hourly operations of generation units based on the unit commitment [1].

There are two key challenges for making an integrated optimization model to schedule the Gencos' outages: 1) the systematic relationship between the short- and the long-term scheduling and 2) the effective coordination between the ISO's objective to reach the maximum reliability and the Gencos' objective to minimize the maintenance cost. Conojo et al. [2] proposed a mixed integer model considering these two challenges without including maintenance interval constraints.

In this paper, a mixed-integer optimization model is developed in which the maintenance intervals constraints and the linkage of short- and long-term operations are considered. Furthermore, to achieve the optimal solution, a specific type of Benders Decomposition technique is applied. Finally, to illustrate the efficiency of the proposed method, a five-bus case study is experimented. It is worth mentioning that the proposed methodology could be promising to solve the large-scale outage scheduling problems within a reasonable time.

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Stochastic multi-commodity facility location based on a new scenario generation technique

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Making decision on Facility location plays a crucial role in supply chain network design. There are generally two specific levels of decisions, strategic and tactical, in the network . The goal in strategical decision is to find the proper locations and their capacities while in tactical level, the objective is to determine the optimal order and the transportation quantities. Using scenario-based stochastic programing techniques in this application are the main contribution of [1] in which these two levels of decisions are simultaneously obtained.
In this research work, a stochastic multi-commodity facility location optimization model are proposed with three new extensions compared to previous research works:

1. apply a new algorithm to efficiently generate scenarios for uncertain correlated demands, this algorithm uses Latin Hypercube Sampling (LHS) and a scenario reduction approach,
2. embed the risk measure using conditional value-at-risk (CVaR) into the optimization model to produce robust policy,
3. consider the customer satisfaction level as a constraint into the optimization model.

Here, the structure of the network contains three facility layers including plants, distribution centers, and retailers. The respective optimization model considers the cost of setup, products' equipment, and transportation related to regional distribution centers and retailers in a single period time.

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AMMCS-2011

Minisymposium: New developments in numerical methods and software for differential-algebraic equations and applications

SS-SDAEA

Organizers:
Andreas Griewank, *Humboldt-Universität zu Berlin (Germany)*
John Pryce, *Cranfield University (UK)*
Ned Nedialkov, *McMaster University (Canada)*

This minisymposium is devoted to recent developments in methods, applications, and software for DAEs and also partial DAEs. Topics can include index determination, consistent initialization, symbolic-numeric techniques for dynamical modeling and simulation, numerical integration schemes, and in particular schemes for high-index DAEs; schemes for structural analysis and integration using automatic differentiation; schemes for event location and its application to hybrid (mixed continuous/discrete) systems; applications of DAEs in optimization, optimal control, circuit analysis, and hybrid dynamic systems.

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Interval Bounds on the Solutions of Semi-Explicit Index-One DAEs

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This work discusses the computation of guaranteed interval bounds on the solutions of nonlinear, semi-explicit index-one differential-algebraic equations (DAEs) subject to a given set of initial conditions and model parameters. Such bounds have applications in uncertainty analysis, state and parameter estimation, safety verification, fault detection, global optimization, validated numerical integration, and controller synthesis. Unfortunately, nearly all available methods apply only to systems described by explicit ordinary differential equations (ODEs). On the other hand, many dynamic systems encountered in engineering applications are best modeled by DAEs.

The proposed approach for bounding DAE solutions combines concepts from differential inequalities and interval Newton-type methods. The first key result is an interval inclusion test which verifies the existence and uniqueness of a DAE solution over a given time step, and provides a crude interval enclosure. This test combines a well-known interval inclusion test for solutions of ODEs (used in standard Taylor methods) with an interval inclusion test for solutions of systems of nonlinear algebraic equations from the literature on interval Newton methods. The second key result is a set of sufficient conditions, in terms of differential inequalities, for two time-varying trajectories to bound the differential state variables; i.e., those state variables whose time derivatives are given explicitly by the DAE equations. Using this result, refined, time varying bounds on the state variables over the given time step are computed using a technique which simultaneously applies differential inequalities to the differential variables and an interval Newton-type method to the algebraic variables.

Based on these key results, an efficient numerical implementation using interval computations and a standard numerical integration code is presented. Strengths and shortcomings of the proposed algorithm are discussed in the context of a five state DAE model for a simple distillation process.

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A Numerical Method with Regularization and Multiscale Properties for Integrating DAEs.

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High index DAE problems have often been solved for control variables in the context of dynamic optimization, by regularizing the constraint, leading sometimes to constraint satisfaction inconsistent with the original problem. In this work we construct a low order numerical integration scheme where variation of an algorithmic parameter reduces the condition number of the Jacobian in certain cases and thus facilitates solution of the high index DAE problem consistent We'll also explore if the variation of the parameter leads to smoothing out of oscillatory and faster variables for usage in multi-scale problems.

The method is essentially a trapezoidal method with a parameterized low-pass filter. We investigate the method both in a traditional time-stepping integrator role and in a direct transcription setting.

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DAE Optimization in Integrated Process Design and Control

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The design of a process plant can have a significant effect on its ability to be satisfactorily controlled. Poor control performance can lead to off-spec product, violation of safety and environmental constraints, and degradation of economic performance. These considerations have led to the development of systematic approaches for analyzing the interaction between plant design and dynamic performance, and developing systematic approaches for incorporation of controllability considerations during plant design. Particularly promising are optimization-based approaches, in which a dynamic model of the plant, typically formulated as a differential-algebraic equation system, is included as constraints within an optimization framework. An economic objective would typically be optimized, subject to equipment constraints as well as path constraints on the dynamic response. The resulting DAE optimization problems are typically large-scale, nonlinear, and may include model discontinuities. This presentation will provide an overview of problem formulations and solution approaches for integrated plant and control design, focusing in particular on approaches followed within our research group. Industrial case studies will be presented and discussed, and avenues for future research identified.

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DAE Index calculation and consistent initialization of multiphysical network models

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Multiphysical network models are used in several applications, for instance in circuit simulation, gas transmission or water transmission simulation. Depending on the modeling level we obtain differential-algebraic equations (DAEs) or systems of partial differential equations and differential-algebraic equations (PDAEs). We first explain the common structure of such problems. Whereas the branch elements of the networks are described by dynamic or static relations between the flow (current/gas/water) and the voltage/pressure, the network graph yields algebraic constraints for the flow. We present a DAE index calculation for such networks basing on the network graph. Furthermore, we introduce an algorithm for computing consistent initial values for the resulting DAE systems exploiting the network structure.

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Pointwise numerical index determination of unstructured DAEs

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The index of a DAE is a measure of the expected difficulties arising when solving it. Given structural properies of a DAE help to determine the index as we know, e.g. from Hessenberg systems or DAEs describing circuit simulations. Automatically generated DAEs coupling various subsystems normally do not show useful structures, but an index determination is absolutely necessary. The index is defined in a "point" belonging to the definition domain of the DAE and depends on this "point". This holds independently of the index definition as examples will show. Among the index definitions the tractability index concept has the following advantages.

- It works with linearizations along arbitrary functions (not necessarily solutions), build by the first derivatives of the given functions.
- The resulting matrices have the same dimension as the original system.
- Choosing widely orthogonal projectors, the whole procedure is unique und step-by-step realizable.
- The index check is done by several constant rank condition checks. This also allows for the detection of critical points, where no index is defined.

In the numerical realization of the matrix sequence it is advantageous to compute the derivatives by means of algorithmic differentiation (AD) because of the higher accuracy. The presented method of numerical index determination may become a basic component on the way to a robust index monitor.

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A Matlab Tool for Structural Analysis of DAEs

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Ned Nedialkov and John Pryce are the authors of DAETS, a C++ code for solving high-index, any order differential-algebraic equations (DAEs). It is based on Pryce's structural analysis (SA) theory and a Taylor series expansion of the solution. Although DAETS can be used for SA, to facilitate our research, we needed a much "lighter", stand-alone tool for SA of DAEs. Over the years, we have been using Matlab to investigate the structure of numerous DAE problems, which resulted in the Matlab DAESA tool (also based on Pryce's SA). The user can specify a DAE in a general form: it can be of high-index, fully implicit, and contain derivatives of order higher than one. DAESA reports the structural index of a DAE, its degrees of freedom, what variables and derivatives need to be initialized (when specifying initial conditions) and what equations and how many times to be differentiated to reduce to an ODE. We outline the theory of Pryce's SA, the implementation of DAESA, and illustrate its capabilities on several examples. Joint work with J. Pryce.

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Pryce pre-analysis adapted to some DAE solvers

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The ODE solver HBT(12)5 of order 12 (Appl. Math. Comput., 211 (2009) 313–328), which combines a Taylor series method of order 9 with a Runge–Kutta method of order 4, is expanded into the DAE solver HBT(12)5DAE of order 12. Dormand–Prince's DP(8,7)13M is also expanded into the DAE solver DP(8,7)DAE. Pryce structural pre-analysis, extended ODEs and ODE first-order forms are adapted to these DAE solvers with a stepsize control based on local error estimators and a modified Pryce algorithm to advance integration. HBT(12)5DAE uses only the first nine derivatives of the unknown variables as opposed to the first 12 derivatives used by the Taylor series method T12DAE of order 12. Numerical results show the advantage of HBT(12)5DAE over T12DAE, DP(8,7)DAE and other known DAE solvers.

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Use of Quasilinearity in Structural Analysis of DAEs

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Ned Nedialkov and John Pryce are the authors of DAETS, a C++ code for solving high-index, any order differential-algebraic equations (DAEs). It is based on Pryce's structural analysis (SA) theory and a Taylor series expansion of the solution. As part of the SA, our algorithms determine the structural index of a DAE, its degrees of freedom, and a block-lower-triangular (BLT) sequence of solving for variables and derivatives in the correct order. This is done as part of consistent initialisation, and also at each integration step for projection on the consistent manifold. The equations concerned are nonlinear in general, and a mix of square (as many equations as unknowns) and under-constrained (fewer equations than unknowns). Our semi-symbolic processing lets us determine whether the unknowns to solve for, in some block subsystem, actually occur linearly (we call this quasilinearity). When a block is both linear and square, it needs no initial values or trial guesses for solution. This reduces the amount of initial data the user must submit, and makes solution more efficient. This is especially powerful when combined with the Dulmage-Mendelsohn decomposition, which yields a finer BLT structure. For the Chemical Akzo problem for instance, an apparently nonlinear 8x8 system reduces thereby to eight linear 1x1 blocks that are trivial to solve. Basic quasilinearity analysis is currently implemented in DAETS, but not yet combined with Dulmage-Mendelsohn. Joint work with Ned Nedialkov.

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Structural DAE Analysis on the basis of the computational graph

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Classically, the properties fo DAEs have been analyzed by examining the Jacobians of the implicit equation with respect to state and velocity and their time derivatives. In some applications like electronic circuits more specific information has been gleaned from the underlying structure of the equations. We attempt to generalize this approach to arbitrary DAEs and to derive systematic procedures for index reduction. The key object is the computational graph that can be generated by automatic differentiation tools.

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Solvability study for Trajectory Prescribed Path Control problems using Pryce's Structural Analysis

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Differential algebraic equations systems (DAEs) appear when trying to solve differential equations subject to constraints. DAEs arise naturally in many modelling applications, such as constrained variational problems, multibody systems, chemical process simulation or electrical circuits. The objective of this paper is to present a formal study of the mathematical solvability of a specific set of DAEs derived from a particular Trajectory Prescribed Path Control (TPPC) problem. InTPPC problems, the DAE system arises from the model of a flying vehicle when constrains are imposed on its trajectory. The TCCP problem studied reflects the aircraft behaviour under Air Traffic Management (ATM) restrictions, such as navigation routes, altitude or speed restrictions, etc. In order to formulate the TCCP problem, the number of constraints has to be equal to the degrees of freedom (DOF) of the equations used to express the motion of the vehicle, thus the DAE system is a closed mathematical problem. However, these constraints cannot have whichever form. Only certain combinations of these constraints ensure that all the DoFs of the equations of motion are closed and moreover, just some of them can ensure that it will exit a unique solution for any given aircraft's initial state It must be ensured that the constraints chosen among all the mathematically possible will be always admitted by the TCI and will drive to a unique solution. This paper shows the elaboration of a set of criteria that permits the correct selection of these constraints among all the possible that can be constructed using the state, control, configuration and environmental variables appearing in aircraft equations of motion. A combination of these constraints according to those criteria must guarantee the solvability of the DAE, i.e., the existence of a unique solution, under any feasible initial condition compatible with the system of equations. These criteria define the sufficient condition for the existence of the solution of a trajectory computation problem in ATM. Pryce's Structural Analysis was used to study the solvability of all the TCCP problems relevant for ATM applications.

Identifying which constraints are compatible with the equations of motion and under which conditions it can be ensured that an output, i.e., the trajectory, can be obtained, are necessary steps to define a generic input to a Trajectory Computation Infrastructure (TCI) used to predict the aircraft trajectory, hence the aircraft intent.

AMMCS-2011

Structured Graph Theory and Applications

SS-SGT

Organizers:
Chinh Hoang, *Wilfrid Laurier University (Canada)*
Kathie Cameron, *Wilfrid Laurier University (Canada)*

For some restricted classes of graphs, one may be able to establish certain structure property and using it to give polynomial time algorithms for problems such as graph coloring, listing paths, etc. In some cases the structure properties are interesting in their own right. The sessions will present recent results in this area.

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Fire Containment in Planar Graphs

Louis Esperet[1], Jan van den Heuvel[2], Frédéric Maffray[3], and Félix Sipma[4]

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Suppose in a graph G a fire starts at some vertex. At every time step, firefighters can protect up to k vertices, and then the fire spreads to all unprotected neighbours. The *k-surviving rate* $\rho_k(G)$ of G is the expectation of the proportion of vertices that can be saved from the fire, if the starting vertex of the fire is chosen uniformly at random. For a given class of graphs $\mathscr{G}$ we are interested in the minimum value k such that $\rho_k(G) \geq \varepsilon$ for some constant $\varepsilon > 0$ and all $G \in \mathscr{G}$ (*i.e.*, such that linearly many vertices are expected to be saved in every graph from $\mathscr{G}$).

In this talk we discuss some results concerning this minimum value for planar graphs and subclasses of planar graphs.

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Robust algorithms for finding triangles in special classes of graphs

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A fundamental issue in algorithmic graph theory is the interplay between the structure of the graphs and the complexity of solving problems on them. Often special structure can yield efficient algorithms; yet, some problems are provably hard in spite of special structure. An intriguing question is where the division between these two cases lies.

Efficiently finding triangles in an arbitrary graph without using matrix multiplication would require a major breakthrough. Hence, a form of complexity lower bound is obtained by showing a given problem is at least as hard as finding triangles. Once finding triangles in a graph is viewed as a fundamental problem, it is natural to ask which classes of graphs are "easy" for finding triangles, and which classes are "difficult".

Algorithms for special classes of graphs can be classified according to the type of assumptions made on the input. Often a special representation of the graph is assumed; for instance, an intersection model or a vertex elimination ordering. Other algorithms require only a promise that the input graph belongs to the class. Another possibility is that there is no promise that the input graph is in the class. When there is no known algorithm for recognizing a class of graphs that is as efficient as a given algorithm to solve a problem on that class, a robust algorithm is most desirable. A *robust* algorithm does not assume the input is in a particular domain; it always produces the correct answer to a problem when the input is in the domain the algorithm is supposed to work on, and when the input is not in the domain the algorithm may either produce the correct output or answer that the input is not in the domain.

We discuss algorithms for finding triangles in graph classes where the time complexity of determining whether a graph is in the class may be larger than the time needed to find a triangle in an arbitrary graph. That is, we want to exploit the special structure of the class without first running a recognition algorithm or being limited to input graphs for which there is a priori knowledge that the graph is in the class. We present efficient robust algorithms to determine whether AT-free (asteroidal triple-free) graphs and EPT graphs (intersection graphs of paths in a tree) are triangle-free (i.e., if the input graph is not in the class, we either produce a triangle of the graph, correctly report that the graph is triangle-free, or determine that the input is not in the class of graphs). In the case of EPT graphs, the recognition problem is NP-complete and the robust algorithm is much harder to obtain than an algorithm that always assumes the input is from the domain.

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Steiner Tree for Fast Data Distribution

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We study the problem of distributing data from a source node to a group of sink nodes along an overlay network of tree topology according to a star-based data distribution protocol. A node represents a host computer which can receive/send data from/to other nodes and has a load balance restriction which limits the maximum number of outgoing channels. Let $w(v,v')$ denote data transfer delay, representing the amount of time to transfer data from node v to node v'; $w(v,v')$ is infinite if the connection from v to v' is not allowed. The star-based data distribution protocol lets a node to send data to all its children one after another, and after all its children receive the data, it signals them to start sending data to their children simultaneously. The overall data distribution time is the amount of time that the source node starts sending data till all sink nodes receive the data, and denoted by $t_T(v_0)$ where v_0 represents the source node and T the overlay network. The problem is to find an overlay network connecting the source node and sink nodes such that its overall data distribution time is minimized. We note that an overlay network allows relay nodes, which are not source or sink nodes, but serve as intermediate nodes.

Let $t_T(v)$ denote the data distribution time that a node v on T starts sending data till all its descendants receive the data. We model $t_T(v)$ by the following function

$$t_T(v) = \max_{v' \in D_T^+(v)} \{ \sum_{v' \in D_T^+(v)} \{w(v,v')\} + t_T(v')\}.$$

where $D_T^+(v)$ denote the set of children of v in T. With this model, $t_T(v_0)$ can be evaluated bottom-up efficiently in terms the number of nodes in T. Using $t_T(v_0)$ as an objective function, we then transform the above overlay network problem to the following combinatorial optimization problem. Given a weighted digraph $G = (V,E,w)$, where V is a node set, E is an edge set, and $w : E \to R^+ \cup \{\infty\}$ is a weight function with $w(e)$ representing the data transfer delay along directed edge e. Also given a source node $v_0 \in V$ and a set of sink nodes $S \subset V, v_0 \notin S$, and a degree constraint b. The problem is to find a rooted tree T of G such that (1) T contains S and v_0 is the root of T, (2) each node of T has at most b children, and (3) $t_T(v_0)$ is minimum over rooted tree satisfying (1) and (2).

This is a specific type of Steiner tree problem on graphs. We see that, when $|V'| = 1$ the problem becomes the shortest path problem. However, when when $b = 1$ and $V' = V$, the problem becomes the shortest Hamiltonian path problem. Therefore, the problem is NP-hard in general.

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The Induced Matching Polytope

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A matching in a graph is a set of edges, no two of which meet a common node. An induced matching in a graph G is a matching M such that no two edges of M are joined by an edge of G; that is, an induced matching is a matching which forms an induced subgraph. I will discuss the induced matching polytope, that is, the convex hull of the incidence vectors of induced matchings. The maximum induced matching problem is NP-hard for bipartite planar graphs, and thus we can not expect a nice description of the induced matching polytope as Jack Edmonds gave for the matching polytope. However, for some classes of structured graphs, such as chordal graphs, there is a nice description of the induced matching polytope.

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Blocking pairs in signed graphs

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A signed graph is a pair (G,S) where G is a graph and S is a subset of the edges of G. A cycle C is said to be even (resp. odd) if it contains an even (resp. odd) number of edges of S. A blocking pair is a pair of vertices x,y such that every odd cycle intersects at least one of the vertices x or y. Blocking pairs arise in a natural way in the study of even cycle matroids as well as in the structure of signed graphs with no odd K5 minors. In this article, we characterize when the blocking pairs of a signed graph can be represented by 2-cuts in an auxiliary graph.

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The complexity of coloring some restricted classes of graphs

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For some fixed k and t, consider the problem of coloring a Pt-free graph with k colors. Recent results have shown that the problem is in P for k = 3, t = 6 and for any k = 1 and t = 5. On the other hand, it is known that the problem is NP-complete for k = 4, t = 9; and k = 6, t = 7. This line of research gives rise to several interesting problems. For example, is there a constant k such that to k-color a P6-free graph is NP-complete? This talk is a survey of recent results in this direction.

AMMCS-2011

Statistical modeling in environmental sciences

SS-SMES

Organizers:
Yulia Gel, *University of Waterloo (Canada)*
Sylvia Esterby, *University of British Columbia - Okanagan (Canada)*

The session aims to discuss the recent trends and advances of statistical methodology, in application to variety of environmental problems ranging from predicting hazardous events to weather and climate prediction.

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Probabilistic Weather Forecasting using the GOP Hierarchical space-time Models

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Nowadays probabilistic weather forecasting becomes increasingly popular among meteorologists and weather users as it enables to produce predictive intervals for a future atmospheric quantity with a prespecified confidence level rather than a single point forecast. This confidence levels are of particular importance for an accurate and reliable assessment of weather uncertainties for risk management tasks. However, typically statistical weather scenarios focus either on capturing a spatial or temporal dynamics. In order to introduce more general non-stationary spatio-temporal effects, we propose to employ a hierarchical Bayesian model to obtain calibrated probabilistic weather forecasts. We illustrate its application in the case of temperature forecast in North American Pacific Northwest.

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Assessment of Trends in Environmental Quality Variables

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With the concern about climate change and the impact of pollutants, researchers have used various statistical methods to identify trends and shifts in temporal records of environmental variables. Monitoring programs which measure environmental quality indicators vary in the length of the records, spatial coverage and consistency of measurements over time. Nonparametric methods for detecting monotonic trends, primarily the Mann-Kendall test, have been widely used for water quality measurements and are also being used for many other environmental variables because of their wide applicability. Approaches which model the form of the trend and permit other features of the data set to be incorporated into the model may also be applied when there is sufficient data. Such approaches will be required when the trend at a location is only one part of the objectives of the statistical analysis. A brief review of methods for trend detection in temporal records at networks of sampling locations will be given. Parametric and nonparametric methods such as LOWESS which are capable of modelling seasonality as well as trend will be compared with nonparametric methods and applied to water quality variables measured in river monitoring networks.

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Statistical tests for dependent hydrological time series

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Studying trends and regime shifts in ice freeze-up and break-up dates as well as ice cover duration on lakes, which are sensitive to the air temperature, provides us useful information about climate change and linkages to atmospheric teleconnection patterns. Such data, however, typically show a positive dependence, which implies that a positive/negative observation tends to be followed by a positive/negative observation in the future. Such dependence among data is known to lead to unreliability of many statistical procedures and tests, making the drawn conclusions inaccurate or even wrong. To overcome the problem, we suggest a number of re-sampling based approaches which take into account the dependence structure of data, for trend and regime shift tracking and provide robust and reliable performance. Currently, we apply our new procedures for the trend and regime shift analysis of freeze-up and break-up dates as well as ice cover observations from Lake Baikal for the period 1869-1996 and Lake Kallavesi freeze-up dates data from 1834 to 1996.

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Monte-Carlo Portmanteau Adequacy Tests for Multivariate Time Series Models

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Multivariate time series models are used widely in econometrics but also in stochastic hydrology for forecasting for multisite riverflow. Multivariate time series also arise in forest fire research for modelling multidimensional environmental variables and predicting forest fire fighting costs. Computational intensive methods based on a Monte-Carlo portmanteau statistical significance test for multivariate time series models have been developed and implemented in a statistical package portes that is available on CRAN. Extensive comparisons using a computer cluster demonstrates that the new method provides more powerful tests than previously used methods both in the asymptotic and finite-sample cases. Our package enables users to rapidly evaluate the p-value for the new tests on modern multicore computers.

AMMCS-2011

Minisymposium on Symmetry in Nonlinear Dynamics: Applications and Numerics

SS-SND

Organizers:
Pietro-Luciano Buono, *UOIT (Canada)*
Manuele Santoprete, *Wilfrid Laurier University (Canada)*
Cristina Stoica, *Wilfrid Laurier University (Canada)*

Symmetry is often found in dynamical models of physical or biological phenomena. It sometimes arises as a modelling assumption based on the spatial features of the phenomena or as a simplification assumption. This scientific session will focus on recent applications of nonlinear dynamics where symmetry plays an important role and also on methods specifically developed for the numerical analysis of symmetric dynamical systems.

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A Poisson Structure and Integrator for the reduced N-body problem

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The general N-body problem is invariant under the symmetry group of translations, rotations, and Galilein boosts. The invariants of this symmetry group can be represented by symmetric block-Laplacian matrices and we show that they posses a Poisson structure. Using this Poisson structure we construct a splitting integrator for the reduced N-body problem. For small N=3,4 this gives an efficient computational method.

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The curved n–body problem

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We study the motion of N–point particles with positive masses interacting under gravitational forces on a surface of constant Gaussian curvature, that we call for short the curved n–body problem. For positive curvature we use the stereographic projection to express the equations of motion, defined originally on the two dimensional sphere, in terms of the intrinsic coordinates of the complex plane endowed with a conformal metric. For the case of negative curvature, we translate the equations of motion defined on the two dimensional hyperbolic sphere to the complex Poincare hyperbolic disk, then, via a suitable isometric fractional linear transformation we translate the problem to the Klein hyperbolic upper half plane and we find the corresponding intrinsic equations of motion. In both cases we obtain the algebraic equations which characterize the relative equilibria. For $N = 2, 3$ we show thes how the existence of different families of relative equilibria.

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Symmetries and dynamics in the 2N-body problem with equal masses: case study of the hip hop family of periodic solutions

Daniel Offin[1],

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The hip hop orbit is an interesting family of symmetric periodic orbits discovered (in 2000 by Chenciner-Venturelli) with the application of global variational methods in the context of gravitational N-body dynamics. Such methods guarantee the existence of a collision free solution of the corresponding Hamiltonian equations of motion which is far from any integrable cases (such as the neighborhood of a relative equilibrium). This solution has a very simple symmetry structure with cyclic spatial symmetry group of order 2 which corresponds to a symplectic equivariant feature of the dynamics in the case of equal masses. It was shown by Chenciner-Venturelli that the angular momentum is not sero, but other qualitative features of this family are not yet fully exposed. We will add to their analysis and show that the family of minimising hip hop orbits has a hidden symmetry which is time reversing, and which resides in the reduced space of the dynamical problem. This additional symmetry then yields a direct product of two reversing symmetries in the reduced space, which may be used to investigate the local dynamics of this globally determined family of periodic orbits. In particular we investigate how this additional symmetry may be used to demonstrate the geometrical fact of hyperbolicity of the local dynamics when an additional assumption of nondegeneracy is placed on the reduced variational equations. The main tool here is a comparison theory for computing intersections of Lagrangian subspaces in the context of the linear dynamics, together with an application of a result by Contreras and Iturraga on the existence of invariant Lagrangian planes.

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A Geometric Analysis of the N-body problem

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In this talk we present a geometric analysis of the n-body problem within the framework of *slice* coordinates (or *roto-vibrational* coordinates). With these coordinates we attain a structure of the equations of motion that allow us to derive certain properties of constant-moment-of-inertia trajectories, which gives a new insight into the discussion of Saari's conjecture. Applications to other aspects of the n-body problem will also be outlined.

The use of slice coordinates to study the dynamics induced by a G-equivariant vector field has been discussed in [4] and has proved fruitful in the analysis of the symplectic structure and momentum maps of general hamiltonian systems in [2][6]. In the case of simple mechanical systems with symmetry one can take advantage of the available structure of the cotangent bundle to obtain additional insight. This has been done in [5], where the link between constant *locked-inertia-tensor* and relative equilibria was analyzed in the sutdy of a generalized *Saari's Conjecture*. In its original form, this conjecture states that constant moment of inertia trajectories in the n-body problem are always relative equilibria. The proof of Saari's conjecture has been elusive even though the converse statement is true in an obvious way. Recent advances on this topic appear in [1][7][3][8][9][3].

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Double Hopf Bifurcations with Huygens Symmetry

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Double Hopf bifurcations have been studied in the generic nonresonant case and in certain strongly resonant cases, including 1:1 resonance. In this paper, the case of symmetrically coupled identical oscillators, motivated by the classic problem of Huygens' clocks, is studied using equivariant normal forms. The focus is on the effects of this Huygens symmetry in modifying the expected dynamics of the system. Although the system is near 1:1 resonance, the symmetry forces this case to have more in common with the nonresonant double Hopf bifurcation than with the generic 1:1 resonant Hopf bifurcation. Many additional features appear, such as in-phase and anti-phase pure mode" solutions that are forced by the symmetry, as well as mixed-mode phase-locked periodic solutions, multi-frequency invariant tori and strange attractors. The escapement paradox is explained.

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Symmetry-based Design and Fabrication of Novel Sensor Systems

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Coupled systems of differential equations are often used as models of physical systems. For example they have been used by Hadley and Aronson to model arrays of Josephson junctions, by Kopell and Ermentrout and Rand to model coupled oscillators and central pattern generators (CPGs) in biological systems, by Pecora and Caroll to investigate synchronization of chaotic oscillators, and, more recently, by Susuki, Takatsuji, and Hikihara to study power grid systems. In these works the symmetry of the network is important in determining the patterns of collective behavior that the system can support. One particular pattern of behavior that is commonly found in symmetric coupled systems is cycling behavior, in which solution trajectories can linger around steady states and periodic solutions for increasingly longer periods of time. In this talk we discuss the existence and stability of heteroclinic cycles in coupled systems and show how they can be exploited to design and fabricate a new generation of highly-sensitive, self-powered, sensor devices. We present theoretical and experimental proof of concept that coupling-induced oscillations located near the bifurcation point of a heteroclinic cycle can significantly enhance the sensitivity of an array of sensors, including: fluxgate magnetometers, electric-field sensors, Superconducting Quantum Interference Devices, and Gyroscopes.

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Stability of stationary fronts in inhomogeneous wave equations

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Models describing waves in anisotropic media or media with imperfections usually have inhomogeneous terms. Examples of such models can be found in many applications, for example in nonlinear optical waveguides, water waves moving over a bottom with topology, currents in nonuniform Josephson junctions, DNA-RNAP interactions etc. This talk considers the effects of (non-local) inhomogeneities on the existence and stability of fronts in nonlinear wave equations.

Homogeneous nonlinear wave equations are Hamiltonian partial differential equations with the homogeneity providing an extra symmetry in the form of the spatial translations. Travelling waves in such system can be viewed as relative equilibria and usually they come in families. Inhomogeneities break the translational symmetry, though the Hamiltonian structure is still present. When the spatial translational symmetry is broken, travelling waves are no longer natural solutions. Instead, the travelling waves tend to interact with the inhomogeneity and get trapped, reflected, or slowed down. As a starting point in understanding this interaction, we study the existence and stability of stationary fronts in the inhomogeneous wave equations.

We look at wave equations with finite length inhomogeneities and assume that the spatial domain can be written as the union of disjoint intervals, such that on each interval the wave equation is homogeneous. The underlying Hamiltonian structure allows for a rich family of stationary front solutions. The existence of those fronts is shown by connecting the unstable respectively stable manifolds of the fixed points in the extremal intervals with the Hamiltonian orbits in the intermediate intervals. So the values of the energy (Hamiltonian) in each intermediate interval provide natural parameters for the family of orbits. After having established existence, the next question is the stability of those stationary fronts. Using Evans function type arguments, we show that changes of stability can only occur at critical points of the length of the inhomogeneity as a function of the energy density inside the inhomogeneity. We also give expressions for the related eigenfunctions in terms of the front solution. With this observation, the stability of the fronts can often be determined by using continuation arguments and Sturm-Liouville theory.

To illustrate how these results can be used to find families of stationary fronts and their stability, we consider a Josephson junction system with a finite length inhomogeneity associated with variations in the Josephson tunneling critical current. This system can be modelled by an inhomogeneous sine-Gordon-type equation and fronts are usually called fluxons. By varying the length of the inhomogeneity, we establish that the system may either not be able to sustain a stationary fluxon or may exhibit various different types of stationary fluxons. If a given system is able to sustain at least one stationary fluxon, there is exactly one stable fluxon, i.e. the system selects one unique stable configuration. Moreover, it is shown that this stable stationary configuration may be non-monotonic; something which is not possible in the homogeneous case. Furthermore, results in the literature on localised inhomogeneities can be recovered as limits of our results. Other applications can be found the DNA/RNAP interactions and if time allows, we will consider this case too.

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Delay-induced primary rhythmic behavior in a two-layer neural network

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In this talk, we construct a two-layer feedback neural network to theoretically investigate the influence of symmetry and time delays on patterned rhythmic behaviors. Firstly, linear stability of the model is investigated by analyzing the associated transcendental characteristic equation. Next, by means of the symmetric bifurcation theory of delay differential equations coupled with representation theory of standard dihedral groups, we not only investigate the effect of synaptic delays of signal transmission on the pattern formation, but also obtain some important results about the spontaneous bifurcation of multiple branches of periodic solutions and their spatio-temporal patterns. Thirdly, based on the normal form approach and the center manifold theory, we derive the formula to determine the bifurcation direction and stability of Hopf bifurcating periodic solutions. Finally, some numerical examples and the corresponding numerical simulations are used to illustrate the effectiveness of the obtained results.

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Bifurcation of symmetric periodic orbits in DDEs and application

Pietro-Luciano Buono[1], Juancho Collera[2],

[1] *University of Ontario Institute of Technology, luciano.buono@uoit.ca*
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I will be discussing the symmetry-breaking bifurcations from periodic solutions with spatio-temporal symmetries in delay-differential equations. The main theoretical result is an equivariant version of the integral manifold theorem of Hale and Weedermann (JDE 2004) which enables us to apply the bifurcation techniques for symmetric periodic orbits developed by Lamb and Melbourne (Arch. Rat. Mech. Anal. 1998). An application to laser models will also be presented.

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Spacecraft Attitude Control with Internal Momentum Wheels

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The problem of spacecraft attitude control with internal momentum wheels was studied by Crouch from a geometric viewpoint in 1984. Since then it has been a popular problem in geometric control. Despite its popularity, it has rarely been systematically examined from the viewpoint of Lagrange-Routh or Lie-Poisson reduction. Unlike the gas jet thrust, the internal momentum wheels do not change the total angular momentum of the whole system, so it is natural to employ the technology of Lagrange-Routh or Lie-Poisson reduction in order to derive a "simpler" set of equations of motion and then address related control issues related to the system. The main ideas of this approach will be presented in this talk. This is an on-going joint work with R. Bayadi and R. Banavar at IIT, Bombay.

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Symmetrical Rearrangement Approach to Constructions of Energy Minimisers

Marina Chugunova[1],

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The fourth order degenerate parabolic equation models the evolution of a thin liquid film on a stationary horizontal cylinder. This equation defines a generalized gradient flow for an energy that controls the H1-norm. It is shown that for each given mass there is a unique symmetrically decreasing steady state, given by a droplet hanging from the bottom of the cylinder that meets the dry region at the top with zero contact angle. The droplet minimizes the energy and attracts all strong solutions that satisfy certain energy and entropy inequalities. The distance of any solution from the steady state decays no faster than a power law. In collaboration with: Almut Burchard and Benjamin K. Stephens.

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An integrable system from complex geometry.

Alex Castro[1],

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Two dimensional complex analysis is even richer geometrically than the one dimensional theory. The boundaries of smooth domains are real 3-manifolds equipped with a contact distribution, and a (conformal) subriemannian metric. These structures are obtained by restricting the ambient Cauchy-Riemann operator to the boundary of the domain. Moreover people like 'E. Cartan. J. Moser, S-S-Chern, C. Fefferman, H. Jacobowitz,Bill Goldman etc. to name a few names, have all looked also at a special class of curves intrinsically attached to these structures, called "chains." Richard Montgomery and I studied similar structures, and curves by considering the three sphere S^3 (as the boundary of the unit ball in $\mathbb{C}^2$) and a family of deformations of the Cauchy-Riemann operator there. To our surprise, the system of ODEs describing the "chains" is integrable, and much of the qualitative behavior of these curves can be described by using Berry phases.

AMMCS-2011

Minisymposium: Progress and Prospects in Model-Based Scientific Software Development

SS-SSD

Organizers:
Christopher Anand, *McMaster University (Canada)*
Spencer Smith, *McMaster University (Canada)*
Diane Kelly, *Royal Military College (Canada)*
Jacques Carette, *McMaster University (Canada)*

This minisymposium will examine recent progress and potential new directions in using model-based development to improve the quality of scientific software.

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Model-based Engineering Design and the Influence of Symbolic Computation, Part I

T. Lee[1]

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The perspectives and needs of "engineering computation" arguably differs from that of "scientific computation." The former stresses a broader technical objective for which the mathematical models and their predictions contribute insight and analytical information. The goal of the latter is the accurate and efficient solution of the inherent mathematical problem itself. Recently, the engineering community in mainstream industry has been actively developing new modeling techniques to increase design confidence and reduce product development time. One of the most significant drivers of this change is the emerging practice of Model-Based (Engineering) Design or MBD. This is not a general concept but a specific technique used in automotive, aerospace, and other precision equipment industries. It consists of the development of high-fidelity "physical models" (the word physical here ironically means mathematical models and not real models of metal, plastic, or clay), which form the foundation for a series of simulation exercises within a purely virtual environment, but also in mixed virtual and hardware. Through such simulations, not only can one identify hazards in design but ultimately identify key parameter values for optimal performance which will then reflect back on choices for parts, manufacture, etc. Prior to MBD, typical design required multiple builds of actual prototypes which then were exercised with real loads and iterations. For cars, this is a very expensive and time consuming process. For aircraft and spacecraft, this is virtually impossible.

Recent developments in MBD is taking the basic idea and enhancing its effectiveness in the key areas of increased model fidelity (more detail), faster model development time, and sufficient execution speed for hardware-based simulations. The need for such improvement is driven by increasing complexity brought on by new products such as Hybrid Electric Vehicles (HEV) that have considerably more components, computer control, and design sensitivities. One of the most interesting trends in the quest for better MBD is the exploration of symbolic computation techniques in model formulation and code generation. The basic idea is simple. Symbolic computation can efficiently manipulate the mathematical expressions of complex equation sets that emerge from automated dynamic model development algorithms. Using basic symbolic operations such as cancellations, multiplications with 1s or 0s, identities, etc., much of the spurious calculations that other non-symbolic formulation techniques simply carry through the iteration can be identified and cleared away prior to expensive iterations. Secondly, by always preserving the mathematical structure of the models in explicit algebraic form, it is easier to implement more sophisticated formulation techniques to deal with more complex system topologies. Finally, specific techniques of code generation (from mathematical expressions to target languages used in engineering) have shown to have enormous benefits in accelerating real time simulation performance. Consequently, symbolic computation-driven simulation has become one of the most promising techniques for a range of key industries.

This presentation will present an overview of the key symbolic computation techniques and case studies from industries. It will use Maple and the MapleSim simulation software as the computation framework.

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Model-based Engineering Design and the Influence of Symbolic Computation, Part II

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The perspectives and needs of "engineering computation" arguably differs from that of "scientific computation." The former stresses a broader technical objective for which the mathematical models and their predictions contribute insight and analytical information. The goal of the latter is the accurate and efficient solution of the inherent mathematical problem itself. Recently, the engineering community in mainstream industry has been actively developing new modeling techniques to increase design confidence and reduce product development time. One of the most significant drivers of this change is the emerging practice of Model-Based (Engineering) Design or MBD. This is not a general concept but a specific technique used in automotive, aerospace, and other precision equipment industries. It consists of the development of high-fidelity "physical models" (the word physical here ironically means mathematical models and not real models of metal, plastic, or clay), which form the foundation for a series of simulation exercises within a purely virtual environment, but also in mixed virtual and hardware. Through such simulations, not only can one identify hazards in design but ultimately identify key parameter values for optimal performance which will then reflect back on choices for parts, manufacture, etc. Prior to MBD, typical design required multiple builds of actual prototypes which then were exercised with real loads and iterations. For cars, this is a very expensive and time consuming process. For aircraft and spacecraft, this is virtually impossible.

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The structure of typed generic code generators

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Now that the feasibility of writing complex typed code generators has been established, along with the creation of a toolset for writing typed code generators, we need to understand how to structure and modularize these new programs. Through the investigation of several program families (generally arising from mathematical software), we have built up a methodology for this task. This methodology will be outlined, as well as several of the key ingredients which make this feasible: abstract interpretation, abstract algebra, partial evaluation, and compile-time symbolic computation. One important feature of our approach is that it relies on (carefully) mixing existing techniques rather than on "new" tools.

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A Family Approach For Scientific Computing Software

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This paper describes a Family Approach for developing Scientific Computing Software (FASCS), illustrated via examples from a family of finite element analysis programs. FASCS is the first methodology to apply a family approach to develop Scientific Computing (SC) software, where all stages in both the domain engineering phase and the application engineering phase are included. The motivation of FASCS is to improve the overall quality of SC software, including reusability, usability, reliability and maintainability. In addition, the challenges for SC software, such as unknown solution challenge, and the characteristics of professional end user developers are also considered.

The methodology includes systematically eliciting, analyzing and documenting common and variable requirements for a program family, using a Goal Oriented Commonality Analysis (GOCA). GOCA proposes two layers of modeling, including the theoretical model and the computational model, to resolve the conflict between the continuous mathematical models that represent the underlying theories of SC problems and the discrete nature of a computer. In addition, the theoretical model and computational model are developed to be abstract and documented separately to improve reusability. Explicitly defined and documented terminology for models and requirements are included in GOCA. The terminology helps avoid ambiguity, which is a potential source of reduced reliability. The traceability of current and future changes is used to potentially improve reusability and maintainability.

FASCS also includes a Family Member Development Environment (FMDE) for the automatic generation of family members. FMDE is apparently the first complete environment that facilitates automatically generating variable code and test cases for SC program families. The variable code for a specific member of the program family can be automatically generated from a list of variabilities written in a Domain Specific Language (DSL), which is considerably easier than manually writing code for the family member. Some benchmark test cases for the program family can also be automatically generated.

A new technique, Computational Variability Test (CVT) is proposed to partly address the unknown solution challenge for SC software. CVT is based on the fact that testing the program family can be performed on the same computational domain with different computational variabilities, since both family members and test cases can be automatically generated. This provides partially independent implementations for which test results can be compared to detect potential flaws.

Nonfunctional requirements, especially nonfunctional variable requirements, are rarely considered in the development of program families. To the knowledge of the author, nonfunctional variable requirements have never been considered in the development of SC program families. Since some nonfunctional requirements are important for SC software, FASCS includes a process using the Analytic Hierarchy Process, a decision making technique, to rank nonfunctional variable requirements and select appropriate components to fulfill the requirements. This process can also be used for ranking nonfunctional goals to select the appropriate numerical technique to solve the continuous mathematical model.

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MRI Velocity Imaging: A Case Study in Symbolic Code Generation

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In this case study, we will describe the problem of reconstructing velocity fields from Magnetic Resonance Imaging data, and use it as a case study to demonstrate the performance advantages in using symbolic code generation.

To that end, we briefly review the physics of MRI in general and velocity imaging in particular, the fundamental challenge in making experiments fast enough to satisfy clinical requirements, and the approach we take to reconstructing accurate velocity profiles with drastically undersampled data, including novel regularization of the underlying inverse problem. We then describe how this transforms a data collection problem into a large computational problem, requiring significant use of parallelism.

To solve the problem of parallel inverse problem generation, we take advantage of symbolic computation, and describe our prototype system of symbolic computation, which nevertheless incorporates novel features which suit it to the generation of efficient derivative calculations given an objective function (with regularizing penalty functions).

We show how parallelization and other optimizations are encoded as rules which are applied automatically rather than schemes which need to be implemented by the programmer in the low-level implementation; and we contrast the way in which symbolic computation leads naturally to automatic test and performance benchmark generation to the conventional way of solving such problems.

Finally, we present performance results, both in terms of numerical results and computational performance.

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MRI Velocity Imaging: A Novel Application of Physical Units to Type Safety

C.K. Anand[1], M.Moghadas[1], J.L.M.Pavlin[1]

[1] *McMaster University, Canada, {anandc,maryamm,pavlinjl}@mcmaster.ca*

In this case study, we will describe Magnetic Resonance Imaging in general and the problem of reconstructing velocity fields in particular, with particular attention to the types of programming errors which arise in this domain, and how adding physical units to the type system can eliminate some of these errors.

To that end, we review the physical units arising in MRI and MRI velocity imaging, and list the common sources of error, explain the consequences of these errors in terms of unsafe diagnoses, and identify the errors which are associated with mismatches in physical units.

Next, we describe the standard methods of incorporating physical units into type systems, for existing languages, the extensions to those methods and the purpose of those extensions. We will then describe a dependent type system incorporating both standard and extended physical units in our prototype symbolic computation environment. We will also discuss the practicality of encoding this type information in existing type systems, specifically, in C and in Haskell.

Finally, we show that most of the potential errors are identified by our type system and flagged for the programmer to correct.

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Degradation of Accuracy in Computational Code

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When developing scientific software, accuracy is a constant concern. The degredation of output accuracy is due to, in-part, the finite bit-precision of floating point variables used in the computation. Individual variables can differ in their sensitivity to changes in the fidelity of their representation, and determining that sensitivity can allow us to fine-tune their representational precision. By increasing precision for sensitive variables and decreasing precision for less sensitive variables, it is possible to improve both the output accuracy and computational performance of scientific codes.

The traditional techniques for such analysis range from analyzing the effect of uniform changes to the rounding mode, compiler flags, and data-types, to static analysis techniques using a combination of interval arithmetic and symbolic analysis, to stochastic simulations and monte-carlo arithmetic. More modern techniques in software engineering, such as dynamic invariant detection and design recovery, have yet to be applied to the scientific software domain. In our preliminary study, we examine the effectiveness of such techniques for the specific problem of determining variable sensitivity to changes in the precision of their representation on a variety of open-source and in-house scientific software. We hope that such an examination can indicate the direction of further research in the development of new tools and techniques for automating the identification of precision sensitivity.

AMMCS-2011

Minisymposium: Theory and Applications in Finance

SS-TAF

Organizers:
Joe Campolieti, *Wilfrid Laurier University (Canada)*
Nick Costanzino, *Wilfrid Laurier University (Canada)*
Roman Makarov, *Wilfrid Laurier University (Canada)*

The goal of this minisymposium is to provide a forum for a fruitful exchange of ideas between academics and practitioners actively involved in cutting-edge research areas which bridge the fields of mathematics and finance. Some research topics include risk management, market microstructure, derivatives pricing and hedging, credit risk modeling and quantitative methods in finance.

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Analysis of contingent capital bonds in Merton-type structural models

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[2] *University of Western Ontario*

Contingent capital bonds (CCB) are securities which "begin life" as subordinated debt, and convert to equity if the issuing firm becomes financially distressed. CCB have recently begun to attract attention as a means to shift the cost of supporting distressed financial institutions from taxpayers to shareholders, thereby enforcing "market-based" discipline. At the present time, however, the discussion surrounding CCB has been largely heuristic. In this talk we attempt, via Merton-type structural models, to shed theoretical light on two fundamental issues regarding CCB. The first is their cost (i.e. par yield), which we find to be surprisingly cheap. Indeed overall debt costs are reduced when CCB are introduced to the capital structure. The second issue we investigate is how CCB respond to changes in fundamental parameters such as leverage and volatility. We find that the answer to this question depends critically on the conversion price, and different prices (for example fixed versus market-based) lead to radically different behaviour.

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A Wiener-Hopf Monte-Carlo simulation technique for Levy processes

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We develop a completely new and straightforward method for simulating the joint law of the position and running maximum at a fixed time of a general Levy process with a view to application in insurance and financial mathematics. Although different, our method takes lessons from Carr's so-called 'Canadization' technique as well as Doney's method of stochastic bounds for Levy processes. We rely fundamentally on the Wiener-Hopf decomposition for Levy processes as well as taking advantage of recent developments in factorization techniques. We illustrate our Wiener-Hopf Monte-Carlo method on a number of different processes, including a new family of Levy processes called hypergeometric Levy processes. Moreover, we illustrate the robustness of working with a Wiener-Hopf decomposition with two extensions. The first extension shows that if one can successfully simulate for a given Levy processes then one can successfully simulate for any independent sum of the latter process and a compound Poisson process. The second extension illustrates how one may produce a straightforward approximation for simulating the two sided exit problem. This is joint work with A.E. Kyprianou, J.C. Pardo and K. van Schaik.

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Mean-Variance Hedging for Path-Dependent Options

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In the paper we consider the problem of hedging of path dependent options. Under the assumed dynamic of the underlying security the market is complete, and hence options can be hedged perfectly by trading continuously a replicating portfolio. However, if we assume, as is the case in practice, that this portfolio can be re-balanced only at discrete time intervals, perfect hedging through a self-financing strategy is not feasible. In the paper we consider hedging strategies that minimize the local risk, which we quantify by using the conditional second moment of the cost increment under the measure P. This approach has been proposed and developed by Föllmer and Sondermann (1986) and Föllmer and Schweizer (1988), but we specialize it to path-dependent options.

In the context of a single-period problem, we show that for European contracts the variance-optimal hedging method and the delta hedging strategy produce errors that are of the same magnitude when the hedging period converges to zero. However, for path-dependent options, even with smooth payoff functions, the mean-variance strategy is always superior when compared with the delta hedging. The latter result has been obtained for a class of payoffs that include Asian options, but the main insight it provides is applicable to all path-dependent options. Based on this analysis we propose a correction to the delta hedging that does not require knowledge of the P measure. Using numeral examples, we also show that for options with less regular payoffs the advantage of using the mean-variance strategy is even more significant.

References

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Did CDS Trading Improve the Market for Corporate Bonds?

Sanjiv Das[1], Madhu Kalimipalli[2], Subhankar Nayak[2],

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Financial innovation through the creation of new markets and securities impacts related markets as well, changing their efficiency, liquidity and pricing error. The credit default swap (CDS) market was undoubtedly one of the salient new markets of the past decade. In this paper we examine whether the advent of CDS trading was beneficial to the underlying bond markets. We employ econometric specifications that account for information across CDS, bond, equity, and volatility markets. We also develop a novel methodology to utilize all observations in our data set even when continuous daily trading is not evidenced, because bonds trade much less frequently than equities. Using an exhaustive sample of CDS and bond trades over 2002â2008 we find that the advent of the CDS was largely detrimentalâbond markets became less efficient, evidenced greater pricing errors and experienced lower liquidity. These findings are robust to various slices of the data set and specification of our tests.

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Nonlinear FBSDEs related to quadratic term-strucutre models

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We consider existence and uniqueness results for some nonlinear forward-backward stochastic differential equations (FBSDEs) related to quadratic term-structure models of interest rates. The forward component of the FBSDE is a Gaussian diffusion or an affine diffusion. We also investigate the case of FBSDEs related to affine term-structure models where the forward component of the FBSDE is a Wishart process.

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Valuing Guaranteed Withdrawal Products with Continuous Management Fee

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In this article, we investigate a particular guaranteed withdrawal benefit product where the underlying fund is driven by two classes of diffusive processes: (i) local volatility and (ii) stochastic volatility. Guaranteed withdrawal benefit products are popular programs offered by many financial institutions to retail clients. An investor provides an upfront investment, which is invested by the financial institution in a fund. The fund tracks the return of an equity or bond index or a basket of the two. To manage this fund, a management fee is withdrawn daily (this will be approximated as withdrawal continuously). In exchange, the investor receives fixed regular payments drawn from the fund. By rewriting the guarantee as an Asian option, and through two measure changes and a dimensional reduction the problem is written in terms of two-dimensional PDE. The PDE is solved by using ADI methods whereby the correlation terms are treated explicitly while other operators are split. We will present numerical examples and discuss issues associate with calibrating stochastic and local volatility surfaces for equity funds.

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Optimal portfolios Regime switching

Luis Seco[1],

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This talk discusses the problem of portfolio optimization when the underlying assets have returns that are not normally distributed; instead, several versions of regime switching methodologies are discussed and compared. Empirical results using hedge fund returns will also be presented.

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IPO Pricing and Wealth Allocation

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This study examines wealth allocation between IPO issuers and subscribers using a new measure inspired by Purnanandam and Swaminathan [2004. Are IPOs really underpriced? Review of Financial Studies 17, 811-848]. We show that underwriters persistently set offer prices so that more than 70% of the total value realized in the IPO process goes to the issuers. Thus, our findings suggest that underwriters favor issuers over subscribers. We further examine determinants of wealth allocation and find that the level of market sentiment and underwriter quality are positively related to allocation to the issuers, whereas the change in sentiment and information asymmetry are negatively related to this allocation.

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Cost Efficiency: Same bang for fewer bucks

Phelim Boyle[1],

[1] *School of Business, Wilfrid Laurier University*

This talk builds on the preference free framework of Dybvig (1988a,b) and Cox and Leland (1982,2000) to analyze dynamic portfolio strategies. We provide an explicit representation of the lowest cost strategy (or "cost-efficient"strategy) and of the most expensive strategy to achieve a given payoff distribution. We explain the deep connections between cost efficiency and anti monotonicity. Our results are illustrated in the Black Scholes setting where we derive new strategies that dominate some well-known option contracts. We extend the approach to deal with additional state-dependent constraints. Explicit solutions are provided and illustrated with examples.

AMMCS-2011

Minisymposium: Numerical Methods for First and Second Order Fully Nonlinear PDEs

SS-VS

Organizers:
Xiaobing Feng, *University of Tennessee (USA)*
Chiu-Yen Kao, *The Ohio State University (USA)*
Ying Wang, *University of Minnesota (USA)*

Since the notion of viscosity solutions was introduced in the early 1980s by Crandall and Lions, it has been successfully developed into a beautiful PDE theory for first and second order fully nonlinear PDEs over the past thirty years. Parallel to the development of the PDE theory, research on design, analysis and implementation of novel numerical methods and algorithms for computing viscosity solutions has been very active, especially in the recent years. Significant progress and advance have been made in this difficult and dynamic research area. The aim of this minisymposium is to bring a group of active researchers in this area to exchange ideas and to present their latest research results in developing numerical methods and algorithms for computing viscosity solutions of a wide class of nonlinear PDEs including Hamilton-Jacobi equations, conservation equations, Monge-Ampere type equations, and Hamilton-Jacobi-Bellman equations.

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Finite element methods for the Monge-Ampere equation

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The Monge-Ampere equation is a fully nonlinear second order PDE that arises in various application areas such as differential geometry, meteorology, reflector design, economics, and optimal transport. Despite its prevalence in many applications, numerical methods for the Monge-Ampere equation are still in their infancy. In this talk, I will first discuss the inherent difficulty of solving this problem and briefly review the numerical literature. I will then discuss a new approach to construct and analyze several finite element methods for the Monge-Ampere equation in a unifying framework. As a first step, I will show that a key feature in developing convergent discretizations is to construct schemes with stable linearizations. I will then describe a methodology for constructing methods that inherit this trait and provide two examples: C0 finite element methods and discontinuous Galerkin methods. Finally, I will end the talk with some applications, further extensions, and some open problems.

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A local discontinuous Galerkin method for directly solving Hamilton-Jacobi equations

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In this talk, we will present a new local discontinuous Galerkin method to directly solve Hamilton-Jacobi equations. The scheme is a natural extension of the monotone scheme. For the linear case with constant coefficients, the method is equivalent to the discontinuous Galerkin method for conservation laws. Thus, stability and error analysis are obtained under the framework of conservation laws. For both convex and non-convex Hamiltonian, optimal $(k+1)^{th}$ order of accuracy for smooth solutions are obtained with piecewise k^{th} order polynomial approximations. The scheme is numerically tested on a variety of one and two dimensional problems. The method works well to capture sharp corners (discontinuous derivatives) and have the solution converges to the viscosity solution.

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An Adjoint State Method for Numerical Approximation of Continuous Traffic Congestion Equilibria

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The equilibrium metric for minimizing a continuous congested traffic model is the solution of a variational problem involving geodesic distances. The continuous equilibrium metric and its associated variational problem are closely related to the classical discrete Wardrop's equilibrium. We propose an adjoint state method to numerically approximate continuous traffic congestion equilibria through the continuous formulation. The method formally derives an adjoint state equation to compute the gradient descent direction so as to minimize a nonlinear functional involving the equilibrium metric and the resulting geodesic distances. The geodesic distance needed for the state equation is computed by solving a factored eikonal equation, and the adjoint state equation is solved by a fast sweeping method. Numerical examples demonstrate that the proposed adjoint state method produces desired equilibrium metrics and outperforms the subgradient marching method for computing such equilibrium metrics.

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Admissibility criteria for compressible potential flow

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We consider admissibility conditions for compressible potential flow, a model for inviscid compressible irrotational fluids consisting of a continuity equation coupled to a Hamilton-Jacobi equation. We show weak-strong uniqueness: if a classical (Lipschitz density and velocity) solution exists, then it is unique in the class of weak essentially bounded solutions. We also show that compression shocks are admissible in our sense while expansion shocks are not. The question of finite speed of propagation will be discussed.

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Analysis and numerical approximation of viscosity solutions with shocks

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We consider a class of Hamilton-Jacobi euqations that represents the propagation of fronts with speed that is a nonlinear function of the signal. The equations contain a nonstandard Hamiltonian that allows the presence of shocks in the solution and these shocks propagate with nonlinear velocity.Shock waves can be formed in finite time from continuous initial data. The new class of Hamilton-Jacobi equations arise from the convective part of a general Fokker-Planck equation ruled by a non-negative diffusion function that depends on the unknown and on the gradient of the unknown. We explore the main features of the solution of the Hamilton-Jacobi equations and propose a suitable fifth order finite difference numerical scheme that approximates the solution in a consistent way with respect to the solution of the associated Fokker-Planck equation. We present a set of numerical results performed under different piecewise constant initial data with compact support for specific equations including the one a two dimensional relativistic heat and porous media Hamilton-Jacobi equations.

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RECOVERY OF HIGH FREQUENCY WAVE FIELDS FROM PHASE SPACE BASED MEASUREMENTS

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Computation of high frequency solutions to wave equations is important in many applications, and notoriously difficult in resolving wave oscillations. Gaussian beams are asymptotically valid high frequency solutions concentrated on a single curve through the physical domain, and superposition of Gaussian beams provides a powerful tool to generate more general high frequency solutions to PDEs. An alternative way to compute Gaussian beam components such as phase, amplitude and Hessian of the phase, is to capture them in phase space by solving Liouville type equations on uniform grids. In this work we review and extend recent constructions of asymptotic high frequency wave fields from computations in phase space. We give a new level set method of computing the Hessian and higher derivatives of the phase. Moreover, we prove that the kth order phase space based Gaussian beam superposition converges to the original wave field unaffected by the presence of caustics.

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A multiscale method for coupling network models and continuum equations in porous media

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We propose a numerical multiscale method for coupling a conservation law for mass at the continuum with a discrete network model that describes the microscale porous media. We aim at the potential application of porous media flow; in this work, we focus on coupling the pressure equations. Network model is discretized on the scale of grains comprising the rock. While it represents a detailed model for multiphase flow, discretizing a larger volume of interest would result in a too large of a system to solve. On the other hand, we assume that over the same physical domain there is an equivalent mass conservation equation at continuum which can be solved much more efficiently *if the equation is explicitly given*. Our coupling method uses simulations on the local network to evaluation the continuum equation and thus solve for the pressure in the domain. We allow nonlinearity in the network model as well as the mass conservation equation. Convergence of the coupling method is analyzed. In the case for which classical homogenization applies, we show convergence of our multiscale solutions to the homogenized equations.

CONTRIBUTED SESSIONS

AMMCS-2011

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Graphs and Demonic Semantics

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Graphs are usually used in computer science to represent programs, automata and Turing machines. These graphs are composed of vertices connected by oriented arcs. Vertices represent control nodes and arcs represent possible transitions of control between commands. Graphs have been used by many authors [1][3], they were introduced with different purposes and defined in connection with the descriptions of algorithms or programs.

We use the same approach as Schmidt and Ströhlein [1][2][3]; they defined a relational program as being a quintuple made of a situation graph, a flowgraph, a relational homomorphism, an input relation and an output relation (for more details see Chapter 10 in [1][3]). Schmidt and Ströhlein have used these notions to treat the total correctness and the partial correctness of programs. By using the same approach as above, we define a *diagram* as being a quadruple constructed of a relation, a set of partial identities disjoint from each other (they have a role identical to the vertices of a graph) and also of two particular partial identities characterizing the input and the output of the diagram.

We consider that nondeterministic programs behave as badly as they can and loop forever whenever they have the possibility to do so. This is the *demonic* approach to the semantics of nondeterministic programs. Our main result is to show that the demonic semantics of a compound diagram is equal to that of the diagram in which each sub-diagram has been replaced by its demonic semantics. This process is repeated until we obtain elementary diagrams to which we apply the results given in our previous work. We will use the monotypes and the residuals.

Our approach uses demonic operations. The operators $\vee$ and serve to give an *angelic semantics*, by defining a program to go right when there is a possibility to go right. The demonic operators $\sqcup$ and $\odot$ do the opposite: if there is a possibility to go wrong, a program whose semantics is given by these operators will go wrong; it's the *demonic semantics* of nondeterministic programs. In this paper we present an approach to analyze the termination properties of these programs.

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Sextic B-spline collocation algorithm for the modified equal width equation

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Sextic B-spline collocation algorithm based on Runge-Kutta fourth order method has been developed for solving numerically the modified equal width wave equation (MEW). This algorithm not only reduces and simplifies the computational work but also results in much more accurate results. Three invariant conditions of motion have been evaluated to determine the conservation properties of migration and interaction of solitary waves. Computation of L_2 and L_∞-error norms shows the better accuracy and efficiency of the generated scheme. A Maxwellian initial condition pulse is also studied. Comparisons have been made with known results whenever available.

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Multi-Level Computational Linguistic Model based on Information Fusion Theory

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Utterly researchers have focused in neurological approaches on the location of points of interest in the brain and its correlation with human language functions at all linguistics levels, much of which has been made in consideration with most popular/spoken languages. Other researchers have focused on the study of language in a higher level of abstraction as irony, speech perception, and other topics emphasizing a psychological approach. However, on the basis that the development of these models should be based on language independence, that in order to build a conceptual basis that allows us to describe the mechanism behind the acquisition and use of any human language. There are countless efforts that must still be performed in order to find some responses that look for Computational Linguistics, either from a psychological, neurological or mixed approach. As such, this research work proposes the construction of a multi-level information fusion approach and integrates it into a computational neurolinguistics model by means of information fusion theory and in this way to correlate acquired data of the human brain imaging in to order to demonstrate its relevance and validation.

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A Time Splitting Semi-Implicit Scheme for Atmospheric Modeling

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The atmospheric models based on the Euler equations for compressible inviscid ideal gas (so-called nonhydrostatic models) describe the processes of very different time and space scales reflecting the variety of phenomena in the Earth's atmosphere. It is well-known that some of these phenomena, such as acoustic waves and small-amplitude gravity waves, have no practical influence on the main processes and can be largely disregarded. However, the structure of the governing equations does not allow simple filtering procedure to eliminate the secondary waves without distortion of the energy significant motions. The only known well-adjusted approximation is based on the hypothesis of hydrostatic balance that filters out three-dimensional acoustic waves and keeps an acceptable level of distortion for principal large-scale phenomena. However, with the recent shift to forecast a broader range of processes, even this approximation was shown to be insufficiently accurate for meso-scale waves.

Since an accurate filtering of fast insignificant waves is not achievable analytically for the required spectrum of the atmospheric phenomena, numerical schemes should incorporate different time discretization for main and secondary processes in order to obtain an efficient numerical solution. Indeed, if one applies a fully explicit time stepping then the solution algorithm at each time step is very simple, but the time step is very small due to the Courant-Friedrichs-Lewy (CFL) condition associated with the propagation velocity of acoustic waves. If, on the other hand, one uses a fully implicit scheme then the time step can frequently be chosen in accordance with the physical requirements of accuracy (about 5-10 min. for models of large- and meso-scale processes), but complex high-dimensional nonlinear problem should be solved at each time step. Since both direct approaches lead to inefficient algorithms, the most popular method in the atmospheric modeling community is semi-implicit, which treat the fast waves implicitly and the slow waves explicitly. Of course, a separation of the processes into the fast and slow parts is rather flexible and different choices give rise to different semi-implicit schemes. The general advantage of the semi-implicit time stepping is that it usually provides the same level of solution accuracy as explicit or implicit schemes with compatible order of operator approximation.

In this research we propose a semi-implicit algorithm with an additional vertical operator splitting for the nonhydrostatic atmospheric model. The designed semi-implicit scheme treats the main linear terms responsible for acoustic and gravity waves in an implicit way, while the remaining terms are discretized explicitly. This approximation is subject to the CFL condition associated with the advection velocity, which allows us to use the time steps of about 3 min., close to acceptable values, but still shorter than it could be chosen to keep the same level of accuracy. A vertical splitting is employed in order to separate more significant gravity waves from almost insignificant ones (the latter being associated with the most part of the vertical spectrum). In this way we can apply more accurate solver for the external and first internal vertical modes, and a simpler and faster solver for the majority of the internal modes. Additionally, for approximation of the advective part we use a discretization on augmented spatial stencil with extended stability, which leads to further increase of the maximum time step up to about 5 min. The last is comparable with the time step required by accuracy considerations in numerical weather prediction models.

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Mathematics and Computation in Biological Sciences and Medicine

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Towards Inter- and Intra- Cellular Protein Interaction Analysis: Applying the Betweenness Centrality Graph Measure for Node Importance

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Objects and relationships between objects are of interest within many Sciences and many other human activities. From a mathematical point of view, *Category theory* studies these in an abstract manner via structures and relationships between them such as via the use of sets and functions. While from a Computer Science point of view, *Graph theory* studies these using the concept of a graph, G, that is defined to be composed of two sets; a set of nodes (also called vertices) V, and a set of edges, E. Relating these two perspectives may be achieved by noticing that an edge may be present or absent between nodes in a graph and that from a mathematical point of view, this is a binary relation. Further abstractions are also possible. This now leads to two problems of interest: *(i)* relating objects and relationships to a suitable representation (such as nodes and edges) and *(ii)* analyzing the representation in order make hypotheses about the original objects of study.

The concrete objectives of this study are to investigate three publicly available biological networks containing protein-protein interaction information in order to determine if such information aids the analysis of two specific biological problems, namely: *(i) inter-* and *(ii) intra-* cellular analysis. There are many avenues of investigation and there is a long history [1- 6]. Results will include an estimate of the importance of proteins for the interaction of inflammatory cells with the blood-brain barrier via the computation of Betweenness Centrality on the selected graphs. Subsequently, they will be validated from a number of differing perspectives; including comparison with *(i)* existing biological results, *(ii)* the literature, and *(iii)* new hypothesis driven biological experiments. Novel therapeutic and diagnostic targets for inhibiting inflammation at the blood-brain barrier in a number of brain diseases including Alzheimer's disease, stroke and multiple sclerosis are expected. In addition, this methodology may also be applicable towards investigating the breast cancer tumour microenvironment.

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A Turing Reaction-Diffusion Model for Human Cortical Folding Patterns and Cortical Pattern Malformations

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In this paper we present a biomathematical model for cortical folding pattern formation in the human brain and apply this model to study diseases involving cortical pattern malformations. Modeling and understanding cortical folding pattern formation is important for quantifying cortical development. Hypotheses concerning brain growth can lead to quantitative biomarkers of normal and abnormal brain growth. Cortical folding malformations have been related to a number of diseases, including autism and schizophrenia.

There is controversy and debate regarding the mechanisms involved in cortical fold formation. Current cortical morphogenesis theories describe folding using tension-based or cellular-based arguments. The axonal tension hypothesis states that cortical folding is a result of tension from corticocortical connections. Axonal tension of highly interconnected regions pulls the walls of the cortex together, forming gyri (folds). Areas with few connections do not have the axonal tension necessary to pull the cortical walls together and result in sulci (valleys). Cellular-based conjectures of cortical fold formation involve a neural progenitor cell called the intermediate progenitor (IP) cell. The intermediate progenitor cell model (IPCM) states that cortical folding is a result of specific patterns of IP cell self-amplification. Regional IP cell amplification leads to regions of neuron amplification in the upper cortical layers, resulting in patterns of gyri and sulci.

Our mathematical model uses a Turing reaction-diffusion system to model cortical folding. Turing systems have been used to study pattern formation in a variety of biological applications. They use an activator and inhibitor and under certain conditions a steady state emerges, causing a pattern to form. We adopt the IPCM mechanism of cortical folding and assume that the activator and inhibitor reactants regulate IP cell production. As the cortex develops, the lateral ventrical (LV) is lined by a layer of proliferative cells called the the ventricular zone (VZ). IP cells are located in a second proliferative layer called the subventricular zone (SVZ). The IPCM suggests subsets of IP cells amplify neurons locally, resulting in gyrus formation. Since the LV and SVZ are critical components in the development of cortical patterning, we model the LV with a prolate spheroid and the SVZ with a prolate spheroid surface. A prolate spheroid is created by rotating an ellipse about its major axis and the major axis of the ellipse corresponds to the major axis of the LV.

We use our model to study how global cortex characteristics, such as shape and size of the LV, affect cortical pattern formation. For example, certain abnormal patterns in human cerebral folding such as enlarged ventricles, lissencephaly (no folds) and polygyria (overproduction of folds) may be due to alterations in the domain shape of the LV. Numerical simulations with our model demonstrate that changes in the focal distance of the prolate spheroid (corresponding to changes in the eccentricity of the LV) result in changes in the location and type of gyral pattern observed. We also apply our model to cortical pattern malformations associated with neural migration disorders. Polymicrogyria is a cortical malformation disease that results in an excessive number of small gyri. We demonstrate that an increase in domain scale can increase the number of sulci and gyri formed. By incorporating LV size and shape, our model is able to elucidate which parameters can lead to excessive cortical folding.

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Dynamic Modeling of Metabolism in Pancreatic β-Cells

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A variety of signaling mechanisms are used to maintain healthy levels of glucose in the blood stream. One of the most important of these mechanisms results in the bi-phasic release of insulin from pancreatic β-cells triggering a series of cellular events involving glucose homeostasis. The second phase of this insulin release, known as the amplifying pathway is not properly understood. There is growing evidence that fuel intermediates from β-cell metabolism act to couple insulin release to blood glucose levels. The cofactor nicotinamide adenine dinucleotide phosphate (NADPH) has been identified as a potential candidate for coupling glucose metabolism to insulin secretion. In this work we develop a kinetic model for the tricarboxylic acid cycle and pathways of its intermediate products based on the previous work of Wu *et al.* [1] and Westermark *et al.* [2]. This ordinary differential equation based model is used to describe the kinetics of the twenty-three enzyme catalyzed reactions describing relevant components of β-cell metabolism. The rate equation for each metabolite [X] is formulated in terms of chemical conservations as follows:

$$\frac{d[X]}{dt} = \sum[X]_{production} - \sum[X]_{consumption}$$

The model was validated against several known results about β-cells [3] and is providing hypotheses to guide further experimental investigation. We are using the model to investigate the role of NADPH and other potential candidates as amplifying signals.

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An Immersed-Boundary Lattice-Boltzmann Model for Microscopic Blood Flow Simulations

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We have developed an immersed-boundary lattice-Boltzmann model (IB-LBM) to simulate red blood dynamics and blood flow behaviors in microcirculation. This model integrates a finite element description of the cell membrane mechanics, the lattice Boltzmann method for the flow field, and the immersed boundary method for cell-flow interaction. This model has also been utilized to examine, for example, red blood cells and aggregates in shear flows, red blood cell migration in straight microvessels, red blood cell trajectories through bifurcated microvessels, multiple-cell suspension flowing in straight microvessels, and effects of membrane elasticity and suspending viscosity on microscopic blood flow behaviors. In this presentation, we will present the model development and recent results of microscopic blood flows in various situations.

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Identification of Transposon Insertion Polymorphisms (TIPs) by computational comparative analysis of next generation personal genome data

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Structural variations (SVs) in genomes are now known as a dominant and important type of genetic variation, which significantly contribute to human diversity and disease susceptibility. The availability of rapidly increasing personal genome sequence data from the use of newer generations of sequencing technologies provides a very rich data source for surveying SVs in humans. Nevertheless, processing the personal genome data in a form of billions of short sequence reads for the identification of SVs represents a very challenging computational task (Ref. [1]). Transposons or transposable elements (TEs) are discrete pieces of DNA that can move within a genome. TEs account for approximately 45% of the human genome and play important roles in the evolution of the genome and regulating gene functions. Among all types of SVs, the identification of transposon insertion polymorphism (TIP) is more challenging than other SVs due to the highly repetitive nature of transposon sequences.

We developed a computational method, TIP-Hunter, to identify TIPs through analysis of next generation personal genome data. TIP-Hunter predicts TIPs via a greedy algorithm based on the mapping patterns of pair-end reads associated with TIPs and other biological characteristics of transposons. We tested the efficiency of TIP-Hunter using a simulated genome containing a set of known TIPs documented in dbRIP (Ref. [2]) and were able to detect about 84% of TIPs with precision of >95%. Using TIP-Hunter to analyze the Solexa pair-end sequence data at deep coverage for six genomes representing two trio families, we identified a total of 3109 TIPs, consisting of 2742, 262, 56, and 49 insertions from Alu, L1, SVA and HERV, respectively, that are absent in the human reference genomes. This list of TIPs has an overlap of 1170 with the 4343 Alu TIPs recently reported by Hormozdiari (Ref.[3]) and 362 with the 781 TIPs documented in dbRIP, leading to a total of 1886 novel TIPs. In addition to the estimated insertion location, TIP-Hunter also provides prediction of transposon subfamily and genotype for each TIP. Our study demonstrates the high efficiency of TIP-Hunter for identification of TIPs, and it represents one of the few comprehensive analyses of TIPs performed so far and reveals an unexpectedly highly level of transposon associated genetic polymorphsim in humans.

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Modeling the effect of topical oxygen therapy on wound healing

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Wound healing is a complex and well orchestrated process that leads to the repair of injured tissue. Oxygen supply is a critical element for the healing of wounds. Clinical investigations have shown that hyperbaric oxygen therapy (HBOT) and topical oxygen therapy (TOT) improve the healing rate of wounds. While HBOT can be administer in all cases, TOT is more suitable to cutaneous wounds. Among many other advantages, TOT does not carry a risk of oxygen toxicity that is associated with HBOT. The underlying reason behind HBOT or TOT improving the healing rate of a wound remain unclear and hence current protocols are empirical. In this paper we present a mathematical model of wound healing that is used to simulate the application of TOT in the treatment of cutaneous wounds. Using the model, we propose an alternative procedure that is capable of better accelerating the process of wound angiogenesis. At the core of our model is an account of the initiation of angiogenesis by macrophage-derived growth factors. The model is express as a system of reaction-diffusion equations, and we present results of simulations for a version of the model with one spatial dimension.

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Enumeration of Saturated RNA Secondary Structures

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RNA (Ribonucleic acid) is an important molecule in the cell, which participates in a lot of basic biological functions. An RNA molecule can be identified by a linear string over RNA alphabet {A (adenine), C (cytosine), G (guanine), U (uracil)}, which is called an RNA primary structure. In secondary structures, RNA bases can form basepairs or single strands. Since the functions of RNA molecules heavily depend on their secondary structures, the study on RNA secondary structures has attracted many researchers.

In this paper, we concentrate on enumeration of saturated RNA secondary structures. A *saturated RNA secondary structure* is an RNA structure such that no basepair can be added. In the Nussinov-Jacobson free energy model [4], an RNA secondary structure is *optimal* if it has the maximum number of basepairs. A t-saturated structure is a saturated structure which contains t fewer basepairs than an optimal saturated structure does. Based on results of enumeration, scientists can choose possible groups or suitable methods for searching. Clote enumerated 0- and 1-saturated structures [2]. However, some of his results are incorrect.

Before enumeration, we first discuss the properties of saturated RNA secondary structures and use skeleton trees to present frame patterns of RNA structures. See Figure 1 for example. According to the number of hairpin loops, we find the generating function for the number of saturated structures with fixed h hairpin loops and b basepairs. Then we enumerate t-saturated structures with n bases. We present the correct result for $t = 1$ as follows and show the result for $t = 2$.

$$Sat_1(n) = \begin{cases} (n-1)(n-3)(n^2+8n+31)/192 & \text{for odd } n, \\ (n-2)(n-4)(n^4+12n^3+68n^2-288n-2304)/9216 & \text{for even } n. \end{cases}$$

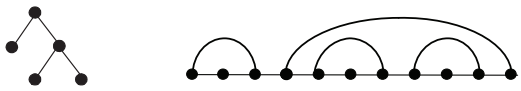

Figure 1: A skeleton tree and the corresponding frame pattern.

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Numerical Experiments on Existence and Non-Uniqueness of Solutions of the Thermistor Problem with Helmholtz Term

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Radiofrequency ablation (RFA) is a minimally invasive therapy form for the treatment of carcinoma, mainly applied in the human liver. An electric current, applied via a needle-shaped applicator, causes heat, which in turn leads to protein denaturation and cell death. A mathematical model of RFA essentially consists of the so-called thermistor problem with an additional Helmholtz term,

$$\partial_t u - \Delta u + \nu u = \sigma(u)|\nabla\varphi|^2, \qquad -\nabla\cdot(\sigma(u)\nabla\varphi) = 0, \tag{1}$$

together with mixed Dirichlet and Neumann boundary conditions for both the temperature u and the electric potential φ, and initial conditions for u [1][2]. The electric conductivity σ can be assumed to be a known function of u. The Helmholtz term νu (where ν can be assumed to be a constant) results from the fact that the liver is pervaded by blood vessels which cause a cooling effect.

Solving (1) is hampered by the fact that $\sigma(u)$ experiences a drastic drop (or even vanishes) as u reaches the boiling point of water. This makes the system become extremely stiff. Performing one step with the most simple scheme suitable for stiff ODEs, the Backward Euler scheme, leads to the steady state form of (1) with an additional Helmholtz term $(1/\tau)u$, where τ is the time step size. Existence of solutions of both the steady-state and the time dependent thermistor problem has been proven by several authors for various settings [3][4]. However, uniqueness results are difficult to obtain, and counterexamples exist for special cases [5]. Also, only very few publications exist about numerical schemes for (1).

The current contribution shows that numerics for (1) is indeed a nontrivial task. Using a spatial discretization by finite elements, our computations show that the nonlinear algebraic equation to be solved in each Backward Euler step does not necessarily admit a unique solution: For some settings, more than one solution is found, while in other situations, although a solution is theoretically known to exist, no solution at all can be identified. Pursuing a homotopy strategy to find a solution for a given time step size τ fails because the solution path exhibits turning points that inhibit the time step size from increasing above a certain value.

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Computational Algebra, Combinatorics and Optimization

CS-CACO

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Computing Bounded Multi-Choose Combinatorics

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Distributing k number of unlabelled balls into n distinct urns is the *n-multichoose-k* problem [1] if each urn can have any number of balls. Here a bounded multi-choose, $M_b(n,k)$, problem where the capacity of each urn is limited to b is considered. Note that if $b = 1$, $M_1(n,k) = C(n,k)$, the conventional *n-choose-k* problem. The concise recursive formula for $M_b(n,k)$ is given and the efficient dynamic programming algorithm to compute the value is presented.

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On algebraic graphs of large girth and their applications

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We study extremal graphs and their applications to coding theory, cryptography, and quantumcomputations. The main object of consideration is a homogeneous algebraic graph defined in terms ofalgebraic geometry in the following way.Recall that a projective space over a field F is a set of elements constructed from a vectorspace over F such that a distinct element of the projective space consists of all non-zero vectors which are equal up to a multiplication by a non-zero scalar. Its subset is called a quasiprojective variety if it isthe set of all solutions of some system of homogeneous polynomial equations and inequalities. An algebraic graph φ over F consists of two things: the vertex set Q being a quasiprojective varietyover F of nonzero dimension, and the edge set being a quasiprojective variety φ in $Q \times Q$ such that$(x,x) \in \varphi$ for each $x \in Q$ and $x\varphi y$ implies $y\varphi x$ ($x\varphi y$ means $(x,y) \in \varphi$). The graph φ is homogeneous (or M-homogeneous) if for each vertex $v \in Q$ the set $\{x|v\varphi x\}$ is isomorphic to some quasiprojective varietyM over F of nonzero dimension. We assume that the field F contains at least 5 elements. If F is finite then the vertex set and theedge set are finite and we get a usual finite graph. The cycle C_t in φ is a sequence $x1,x2,\ldots,xt$ of distinct elements of Q such that $x1\varphi x2, x2\varphi x3, \ldots, xt?1\varphi xt, x1\varphi xt$ are edges of the graph.We define the girth $g = g(\varphi)$ of a graph φ as the length of its minimal cycle. If φ is without cyclesthen $g(\varphi) = \infty$. We study the following two optimization problems: (A) Let Q be a M-homogeneous graph such that $dimM = k$ over F and its girth is a finite number g.What is the minimal possible dimension $v_a(k,g)$ for the variety of vertices?

(B) Let φ be a homogeneous graph of girth $g \geq t$ and $dimM = k$. What is the maximal possibledimension of φ? Problems (A) and (B) are related to each other, in case of finite field we can change the dimensionof Q and φ on their cardinalities and get classical problems on minimal order of regular simple graphof given degree and given girth (analogue of A) and maximal size (number of edges) of the graph with girth $\geq t$ (analogue of B). So (A) and (B) are motivated by the branch of extremal graph theory which studies order of cages,related bounds, cages itself, bounds on maximal number of edges of the graph of given order and girth,and families of graphs of large girth.

We consider an analogue of Tutte's bound and variants of Erd$\acute{}$os even circuit theory forhomogeneous graphs, and define the family of algebraic graphs of large girth over an arbitrary field.Examples of extremal algebraic graphs of bounded dimension are presented. We formulate some openproblems for general homogeneous graphs motivated by classical extremal graph theory.

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Over-correction for multi-level aggregation for Markov chains

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In many application areas including information retrieval, biological modeling and performance modeling of communication systems, the stationary distribution of an irreducible Markov chain is of interest, and is often difficult to compute. The stationary probability vector satisfies the equation $B\mathbf{x} = \mathbf{x}$, subject to the constraints $\|\mathbf{x}\|_1 = 1$ and $x_i \geq 0 \; \forall i$, where B is a column-stochastic matrix. A relatively new approach to solving this problem has been the application of multigrid techniques. The resulting multi-level methods are related to the two-level methods traditionally used to solve such problems, and are based on the multi-level aggregation framework developed by Horton and Leutenegger for Markov chains. While multi-level aggregation methods have shown promise, they typically need to be accelerated in some way in order to achieve suitable convergence .

In this talk we present a simple automatic over-correction mechanism to accelerate multi-level aggregation methods for the computation of the stationary probability vector of irreducible Markov chains. This is motivated by the observation that while the correction typically approximates the error very well in the sense of its "direction", it may not provide a good approximation in the sense of its "size". In the case of a multiplicative correction scheme, which is commonly used for Markov chains, we apply the over-correction technique via componentwise exponentiation of the correction by a small factor $\alpha > 1$, that is recalculated on each level. Numerical experiments demonstrate that this approach can lead to significant speedup of basic multi-level aggregation for Markov chains, at little extra cost.

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An Asymptotically Optimal Two-Stage Algorithm of Classifying Multiple Mutually-Obscuring Positives

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The classic pooling design problem is to identify an unknown set of positive samples among a given large collection of samples by using as few queries as possible. In this talk, we introduce a novel and natural generalization of the well-studied pooling design problem: Consider a set $\mathscr{N}$ of n items which is known to contain k types of positive objects $R_1, R_2, \cdots, R_k$, where $|R_i| \leq r_i$, and the others being negative objects. A query Q can be any subset of $\mathscr{N}$ and $k+1$ possible responses will be given according to the following rules:

- If $|Q \cap R_i| > 0$ for some *unique* i, i.e., Q contains only one type of positive objects, then the response will be "Q is i-positive".
- If Q contains *only negative objects*, then the response will be negative.
- If Q contains *more than one type of positive objects*, then the response can be negative or be i-positive for some i (Q must contain some objects in R_i).

We refer to this problem as the *Multiple Mutually-Obscuring Positives Problem*. Obviously, the classic pooling design problem is the special case of $k = 1$. As for the $k = 2$ case, it is coincident with the well-known puzzle of finding counterfeit coins, where the unknown counterfeit coins can be heavier or lighter than normal coins.

Firstly we provide a test-optimal 2-stage algorithm for this problem. Notably, our strategy is also stage-optimal because theoretical lower bound on the number of queries for any strategies cannot be achieved by 1-stage strategies. Instrumental to the main result is based on a combinatorial structure, (k,m,n)-*selector*, first introduced by De Bonis, G**c**asieniec and Vaccaro [1] in the context of designing efficient trivial 2-stage pooling strategies on the classic pooling design problem. Secondly we propose a new point of view for the mentioned selectors. This enables us to construct the combinatorial tool easily. Probabilistic constructions are provided and numerical results show that our constructions are slightly better than the currently best known result by De Bonis et al. [1].

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Minimal equations of genus two curves over their fields of definition.

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In this paper we study the minimal equation of genus 2 curves over their fields of definition. This problem has been studied by many authors before. An algorithm was suggested by Mestre (93) for genus 2 curves with automorphism group of order 2 and by Cardona (2003) for curves with automorphism group of order ≥ 2. In both these works the locus $C = 0$, where C is the Clebsch invariant, was left out. Furthermore, none of these works guaranties a minimal equation for the curve. We complete both works by treating the case $C = 0$. Furthermore, we obtain a minimal equation in all cases. Our algorithm is implemented and made available to the public. To our knowledge this is the first time that such a complete algorithm is suggested and implemented.

Let k be an algebraically closed field of characteristic zero and C a genus 2 curve defined over k. Then C can be described as a double cover of $\mathbf{P^1}(\mathbf{k})$ ramified in 6 places $w_1, \ldots, w_6$. This sets up a bijection between isomorphism classes of genus 2 curves and unordered distinct 6-tuples $w_1, \ldots, w_6 \in \mathbf{P^1}(\mathbf{k})$ modulo automorphisms of $\mathbf{P^1}(\mathbf{k})$. An unordered 6-tuple $\{w_i\}_{i=1}^6$ can be described by a binary sextic (i.e. a homogenous equation $f(X,Z)$ of degree 6).

Consider a binary sextic, i.e. a homogeneous polynomial $f(X,Z)$ in $k[X,Z]$ of degree 6. *Igusa J-invariants* $\{J_{2i}\}$ of $f(X,Z)$ are homogeneous polynomials of degree $2i$ in $k[a_0, \ldots, a_6]$, for $i = 1,2,3,5$. These J_{2i} are invariant under the natural action of $SL_2(k)$ on sextics. Dividing such an invariant by another one of the same degree gives an invariant under $GL_2(k)$ action.

Two genus 2 curves C in the standard form $Y^2 = f(X,1)$ are isomorphic if and only if the corresponding sextics are $GL_2(k)$ conjugate. Thus the $GL_2(k)$ invariants are functions on the moduli space $\mathscr{M}_2$ of genus 2 curves. This $\mathscr{M}_2$ is an affine variety with coordinate ring $k[\mathscr{M}_2] = k[a_0, \ldots, a_6, J_{10}^{-1}]^{GL_2(k)}$ which is the subring of degree 0 elements in $k[J_2, \ldots, J_{10}, J_{10}^{-1}]$. The *absolute invariants* $i_1 := 144\frac{J_4}{J_2^2}$, $i_2 := -1728\frac{J_2 J_4 - 3J_6}{J_2^3}$, $i_3 := 486\frac{J_{10}}{J_2^5}$, are even $GL_2(k)$-invariants. Two genus 2 curves with $J_2 \neq 0$ are isomorphic if and only if they have the same absolute invariants. If $J_2 = 0$ then we can define new invariants as in [1]. By a point $\mathbf{p} \in \mathscr{M}_\mathbf{2}$ we mean the following $\mathbf{p} := (\mathbf{i_1}, \mathbf{i_2}, \mathbf{i_3})$ if $J_2 \neq 0$ and $\mathbf{p} := (\mathbf{a_1}, \mathbf{a_2})$ if $J_2 = 0$

Problem: Let $\mathbf{p} \in \mathscr{M}_\mathbf{2}$. Determine the field of definition F of $\mathbf{p}$ and find explicitly a genus 2 curve C defined over F which corresponds to p.

We completely solve this problem. Furthermore, the algorithm is implemented it in Maple.

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Waterloo, Canada, July 25-29

On the Bounded Integer Partition

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Partitioning a positive integer n into k parts is an important combinatorial problem, i.e., distributing n unlabelled balls into k unlabelled urns where no urn is empty [1][2]. The bounded integer partition problem is counting the number of partitions where the capacity of each urn is limited to b. Partially ordering bounded partitions of a positive integer forms a graph whose nodes are sets of unlabeled lists. The concise formulae and algorithms for generating the order and size of such graphs are given and analyzed.

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Accelerating linear system solutions using randomization techniques

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We illustrate in this paper how linear algebra calculations can be enhanced by statistical techniques in the case of a square linear system $Ax = b$. Such a linear system is commonly solved using Gaussian Elimination with Partial Pivoting (GEPP) which is implemented in most linear algebra libraries (e.g. LAPACK) resulting in very stable algorithms. However, even though there is no floating-point operation in pivoting, it involves irregular movements of data and the communication overhead due to pivoting can represent up to 50% of the global computational time on some architectures (multicore, GPUs).

We study here an approach based on randomization where the original matrix A is transformed into a matrix that would be sufficiently "random" so that, with a probability close to 1, pivoting is not needed. This randomization is referred to as Random Butterfly Transformation (RBT) in [1]. It consists of a multiplicative preconditionning U^TAV where the matrices U and V are chosen among a particular class of random matrices called *recursive butterfly matrices*. Then Gaussian Elimination with No Pivoting (GENP) is performed on the matrix U^TAV and, to solve $Ax = b$, we instead solve $(U^TAV)y = U^Tb$ followed by $x = Vy$. Note that, since we know that we do not pivot, GENP can be implemented as a very efficient fully BLAS 3 algorithm.

We show that in practice, at most two levels of recursivity are required for butterfly matrices to obtain an accuracy close to that of GEPP. Then the maximum cost for the preconditionning is $\sim 8n^2$ operations where n is the matrix size, which is negligible when compared to the cost of pivoting. For sake of stability we also give the possibility of adding some iterative refinement steps in the working precision where the stopping criterion is the componentwise relative backward error. For matrices that we use in our experiments, we never need more than one iteration. Another observation is that RBT does not change significantly the 2-norm condition number of the initial matrix A.

We describe an RBT solver where the preconditionning and GENP are optimized similarly to [2] in order to take advantage of the latest generation of hybrid multicore/GPU machines. We compare the GFlop/s performance of this solver with that of solvers from the parallel libraries MAGMA and PLASMA.

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Nonlinear quantum optics model for laser-gas interaction in some extreme regimes

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In this talk we are interested in the modeling and simulation of intense and ultrashort electromagnetic fields propagating in a molecular gas. In this goal a Maxwell-Schroedinger system has been proposed in 1 and improved in 2. The electromagnetic field (laser pulse) is modeled by the macroscopic Maxwell equations which are coupled with many time dependent Schr odinger equations using a P.I.C.-like approach. The ab initio description of the laser-molecule interaction allows us to include high order harmonics and nonlinearities. When the gas is ionized, a plasma of free electrons is created inducing a current whose evolution is modeled by a differential equation which is coupled with the Maxwell-Schroedinger system. After discussing some mathematical properties of this system, and its numerical approximation and optimization, we will present some simulations showing the behavior of the model depending on the gas density and on the incoming laser intensity. In particular, self-focusing and defocusing effects will be observed and discussed.

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Adiabatic control of single electron spins in semiconductor quantum dots through the application of Berry phase

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Single electron spin states in a quantum dot can be manipulated by moving the dot adiabatically in a closed loop in the plane of two dimensional electron gas (2DEG). In such a system, in addition to the dynamical phase factor, the dot acquires an additional phase factor, known as the Berry phase. In our previous work [1], we studied the manipulation of single electron spin states through SU(2) spin propagator for GaAs quantum dots where the energy spectra of the dots are degenerate. In this paper, we extend this study to the manipulation of single electron spin states through the scalar Berry phase for InAs quantum dots. Based on both analytical and numerical simulation techniques, we study the manipulation of single electron spin states by controlling the quantum states adiabatically through the application of gate controlled electric fields . Our study has shown that the anisotropic gate potential extends the level crossing (two eigenstates have the same spin) to larger quantum dot radii as well as to larger magnetic fields with the variation of scalar Berry phase. Manipulations of single electron spins through the Berry phase is important since spin quantum states are topologically protected from the environment. The Berry phase generated in semiconductor quantum dots generally induces a quantum spin phase gate during the precession of spins in the plane of 2DEG, providing a number of possible applications in solid state quantum computing.

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On the numerical solution of the convection diffusion equation in the real projective plane.

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We study a mathematical model problem related to fibre suspension flows. These kind of flows arise for example in paper industry. One wants to compute the orientation probability distribution of the fibres in some domain. The fibre is taken to be an infinitely thin rigid rod, hence its orientation can be parametrized by the real projective plane RP^2. In order to solve the orientation distribution it is necessary to study convection diffusion equation on RP^2. As far as we know this has not been numerically treated in the literature before.

In order to formulate the problem we have to use proper Riemannian metric in RP^2 which in our case is the round metric induced by the unit sphere. To discretize the problem we first cover RP^2 with some appropriate coordinate patches. We triangulate these coordinate domains in R^2 in a standard way and use the metric to adjust properly the size of the triangles. We then compute the solution using variational formulation. This is possible although RP^2 is a nonorientable manifold. We will present the results of our computations both in elliptic and parabolic case.

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Plane symmetric domain walls and cosmic strings in bimetric theory

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The field equations for thick domain walls and cosmic strings are solved for plane symmetric space time in Rosen's (General Relativity and Gravitation **4**, 435, 1973)bimetric theory of gravitation. Various physical and geometrical properties of the models have also been discussed.

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Atomic simulation of novel functional materials for radiation medical imaging detectors

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Modeling of physical properties is an integral part of continuous improvement in existing and development of new functional materials. Quantum mechanical firsts-principle simulations, such as the density functional theory (DFT), play an increasing role in this process as they offer a unique possibility to foresee material properties solely on the base of their atomic structure. Our objective is to facilitate improvement of critical properties of materials for x-ray medical imaging detectors by gaining an understanding of fundamental physical mechanisms responsible for degradation of a detector's performance. More specifically, we focus on modeling of defects responsible for poor temporal characteristics of direct conversion x-ray detectors based on lead oxide (PbO), since understanding the origin of these defects holds the key to improvement of the material quality.

Polycrystalline PbO has recently emerged as a favorable photoconducting material for direct conversion x-ray detectors, and the first prototype of a large-area detector has been demonstrated [1]. However, a non-perfect temporal behaviour (image lag and ghosting) due to charge trapping at defects currently prohibit the success of this material in application for direct conversion dynamic detectors.

Using DFT (Wien2k package [2]) it was possible to determine conditions that govern formation of various point defects (vacancies and antisites) and thermodynamic preferences. Also, we identified chemical elements that can be used in order to passivate existing defects (see Fig. 1) by neutralizing electronic traps they introduced. Finally, we address the stability of these complexes.

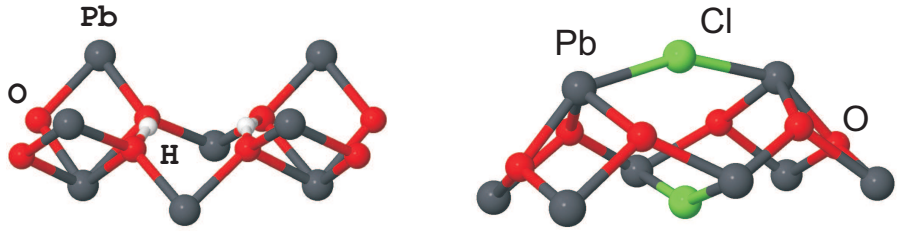

Figure 1: Lowest energy atomic structure of passivated lead and oxygen vacancies in PbO (left and right, respectively).

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Exact Solutions Of Some Linear And Nonlinear Schrödinger Equations Using The Differential Transform Method

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In this paper, we introduced a modification of the differential transform method using Laplace Transform and Padé approximation to obtain closed form solutions of linear and nonlinear Schrödinger equations. It solves the drawbacks in the standard differential transform method. Illustrative examples are presented to show the reliability and simplicity of propose technique.

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Nanoscopic Heat Conduction: Numerical Solutions, Main Features and New Developments

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After a brief description of the constructivist conception in which nanoscopic heat conduction phenomenons are interested for mathematicians, physicists and engineers, the main features of numerical approaches for the solution of nanoscale heat transport problem will be presented. They include elements such as, the possibility of modeling, numerical solutions, closed analytical form solutions and various 1D, 2D and 3D laser heat sources. Then some aspects related to new developments will be discussed. They are related to non Fourier properties of the microscopic/nanoscopic heat conduction with existing laser heat sourses, stability, controllability and the numerical solutions for the novel heat equation. Finally, some concluding remarks will be outlined. Numerical results are presented.

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VIBRATIONALLY AVERAGED LONG-RANGE MOLECULE-MOLECULE DISPERSION COEFFICIENTS FROM COUPLED-CLUSTER CALCULATIONS

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Recent years have seen increasing interest in the structure and dynamics of molecular clusters formed when a chromophore molecule such as CO2, OCS or N2O is solvated by number of He atoms and/or para-H2 molecules. A key experimental probe of their behaviour is the shift of a chromophore's vibrational transition frequency which occurs when the solvent species are attached to it. Such shifts are driven by the changes in the solvent-chromophore interaction potential upon vibrational excitation of the probe molecule.

While 'conventional' supermolecule calculations can often provide realistic predictions of such changes in the potential well and repulsive wall region, they become increasingly unreliable for describing the weak interactions at long range where most of the solvent species in a large cluster are located. It is therefore important to have accurate relative-orientation and monomer-stretching dependent long-range C6, C8 and C10 dispersion coefficients to incorporate into the models for the interaction potential and for its dependence on the chromophore's vibrational state. This paper describes how those coefficients can be obtained from calculated monomer dipole, quadrupole, and octupole polarizabilities for imaginary frequencies, and by making use of the Casimir-Polder relation and angular momentum coupling to extract orientation-dependent quantities. The calculations are performed using a modified version of the ACES2 program system which allows the calculation of dipole, quadrupole and octupole polarizabilities at the EOM-CCSD level, and of static multipole moments using CCSD(T) calculations and adequate basis sets. For each relevant level of the chromophore, vibrational averaging is performed by calculating the imaginary frequency polarizabilities at judiciously chosen geometries and performing a numerical integration using the free-molecule vibrational wavefunction. Subsequent work will involve merging this long-range part of the potential with a short-range part obtained from 'conventional' CCSD(T) calculations and using it in PIMC simulations of cluster behaviour.

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Theoretical Description of Photoelectron Spectra of Biradicaloids

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Chemistry has been categorized and presented as an experimental science for a long time in the history of Science. Until recently, this view has been prominent amongst majority. However, with the invention of quantum mechanics in early 20th century, it has become possible to theoretically predict chemical properties by means of solving the Schrodinger equation. Although exact description of many-body systems, i.e. atoms and molecules, is computationally willful, physicists and chemists have developed approximate methods that are capable of describing the systems with reasonable accuracy with the help of powerful computers. This field of research is widely known as Quantum Chemistry. Among the wave function based electronic structure methods, single-reference coupled-cluster theory has enabled highly accurate description of small-to-medium sized molecules.

However, in certain multi-reference cases such as biradicals, bond-breaking processes and excited states, single-reference coupled-cluster theory fails to provide even a qualitatively correct description. Multi-reference coupled-cluster methods that are applicable to such systems as well as to general open-shell systems are in active development in our group. Also, to be able to make direct and meaningful comparison to the experimental results, electronic structure technique is being coupled to an efficient scheme in order to describe non-adiabatic nuclear dynamics, based on vibronic model Hamiltonians. At this stage, benchmark calculations have been performed for selected biradical systems using the ACES II program. These results when combined with vibronic coupling will be used to simulate the photoelectron spectra of these systems. Application of these methods to transition metal compounds is a prospective goal.

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An efficient parallel numerical method for solving reaction-diffusion partial differential equations based on generalized random trees

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A new parallel numerical algorithm based on generating suitable *random trees* by means of *branching diffusion processes* is proposed for solving reaction-diffusion partial differential equations. Two different approaches are discussed, both requiring generating suitable random trees, governed by a new probabilistic representation of the solution, combined with a Pade approximant for approximating accurately a given divergent series. Such series are obtained by summing the partial contribution to the solution coming from trees with arbitrary number of branches.

The new representation expands largely the class of problems amenable to be solved probabilistically, and is used successfully to develop a generalized probabilistic *domain decomposition* method. Such a method has been shown to be suited for massively parallel computers , enjoying full scalability and fault tolerance. In short, the idea consists of generating only few interfacial values using the probabilistic approach along a given possibly artificial interfaces inside the domain, obtaining approximate values interpolating on such interfaces, and then use such values as boundary data in order to split the original problem into fully decoupled sub-problems.

While classical techniques based on a deterministic domain decomposition exhibits strong limitations in terms of scalability, probabilistic methods are capable of exploit massively parallel architectures since the problem can be fully decoupled. Some examples have been run on a high performance supercomputer, showing a remarkable scalability and performance.

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AMMCS-2011

Applications of Dynamical Systems and Differential Equations

CS-DSDE

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Analysis of neural networks with piecewise constant argument of generalized type

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We shall discuss how to model neural networks by using differential equations with piecewise constant argument of generalized type. These networks have been extensively studied in recent years due to their applicability in solving associative memory, image and signal processing, pattern recognition and so on. As it is well known, applications of neural networks depend crucially on the dynamical behavior of the networks.

In the first part of talk, we describe the structure of biological neurons and artificial neuron model proposed by McCulloch and Pittz. Next, basic properties of differential equations with piecewise constant argument of generalized type will be given. Finally, stability of periodic solutions and equilibria of the systems will be discussed.

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Two Maps and Worldwide Ipod Interest

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There is often a desire to determine if the dynamics of interest are chaotic or not. Since positive Lyapunov exponents are a signature for chaos, they are often used to determine this. Reliable estimates of Lyapunov exponents should demonstrate evidence of convergence; but literature abounds in which this evidence lacks. This paper presents two maps through which it highlights the importance of providing evidence of convergence of Lyapunov exponent estimates. Worldwide ipod interest is then used as a practical example and the results bear semblance to both maps.

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Sparsity Preserved Computation for Matrix Sign Function

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The simulation of the large scale dynamical systems requires large amount of computational power. Thus, reducing the computational cost of these types of simulations deserves attention in the applied mathematics community. A well-known solution method for these types of problems is the model order reduction (MOR), which aims to build an approximate dynamical model of the system with an order significantly smaller than that of the original system. There are several approaches for MOR [1]. In this study, eigenvalue based model order reduction methods based on Matrix Sign Function (MSF) are investigated. These type of methods are based on determination of the dominant poles of dynamical system for approximation [2,3]. To find the dominant eigentriplet of the system matrices, one can use the Matrix Sign Function (MSF) iteratively. MSF behaves like its scalar equivelant. Scalar sign function, extracts the sign of a real number. Similarly, MSF detects the signs of eigenvalues of a matrix and its output is two blocks of identity matrix. The sizes of the first and the second block matrices correspond to the number of positive and negative eigenvalues of the matrix respectively.

In the literature one can find several methods for computation of MSF [4].

The inverse of a square matrix has to be taken explicitly several times in all of these MSF computation algorithms. Therefore, the computational cost of MSF is very high. Mostly, the system matrices of the large scale dynamical systems are very large and sparse. Thus, the inverse becomes full. Hence, it is a challenging problem to find an efficient and sparsity preserving method for the computation of the MSF of the system matrices. In the present work, the MSF required by the model reduction algorithm proposed in [3] is computed by both the Newton-type methods and the integral form methods with sparse approximate inversion [5]. The results are compared in terms of accuracy, sparsity preservation capabilitiy and the computational efficiency.

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On Hurwitz and Schur Connecting-Curves and dense trajectories

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The aim of this work is to give a Hurwitz connecting-curve (which is a family of polynomials) joining any two arbitrary stable polynomials in the set of Hurwitz polynomials with positive coefficients, $\mathscr{H}_n^+$. This and the homotopy of paths allow to prove the existence of a dense trajectory in $\mathscr{H}_n^+$. It implies, by the Mobius map that we can find a connecting-curve in the set of the Schur polynomials, $\mathscr{S}_n$.

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The dynamics of a delayed predator-prey model with state dependent feedback control

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A delayed prey-predator model with state-dependent impulses is investigated for the case of small delay. The boundedness of solutions is analyzed by applying the comparison argument. The sufficient conditions of existence and stability of semi-trivial solution and positive period-1 solution are obtained by using the Poincare map and analogue of the Poincare criterion. The qualitative analysis shows that the positive period-one solution bifurcates from the semi-trivial solution through a fold bifurcation. Numerical simulations are carried out to illustrate the feasibility of main results.

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Synchronized Oscillation and Oscillation-Arrested for Segmentation Clock Gene of Zebrafish

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Somitogenesis is the process during the development of somites. This process is based on the synchronous oscillation of the gene expression of the "segmentation clock genes". In this presentation, we analyze the dynamics for a model with delay on zebrafish segmentation clock-genes which include more intermediate process than other models in gene expression, namely, translation of the clock protein from cytoplasm to nucleus. For this system, an ingenious iteration approach is applied to obtain the global synchronization and global convergence to the unique synchronous equilibrium. On the other hand, for local dynamics, we derive the criteria for the existence of stable synchronous oscillations by using the Hopf bifurcation theory and the center manifold theory. Our analysis provides the basic range of parameters and delay magnitudes for stable synchronous, asynchronous oscillation, and oscillation-arrested dynamics. Based on the derived analytic criteria, further numerical findings are explored to link to the biological phenomena.

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Hadamard factorization of stable polynomials

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The stable (Hurwitz) polynomials are important in the study of differential equations systems and control theory (see [1] and [2]). A property of these polynomials is related to Hadamard product. Consider two polynomials $p,q \in R[x]$:

$$p(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

$$q(x) = b_m x^m + b_{m-1}x^{m-1} + \cdots + b_1 x + b_0$$

the Hadamard product $(p * q)$ is defined as

$$(p * q)(x) = a_k b_k x^k + a_{k-1}b_{k-1}x^{k-1} + \cdots + a_1 b_1 x + a_0 b_0$$

where $k = \min(m,n)$. Some results (see [3]) shows that if $p,q \in R[x]$ are stable polynomials then $(p * q)$ is stable, also, *i.e.* the Hadamard product is closed; however, the reciprocal is not always true, that is, not all stable polynomial has a factorization into two stable polynomials the same degree n, if $n \geq 4$ (see [4]).

In this talk we will give some conditions to Hadamard factorization existence for stable polynomials.

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Takens-Bogdanov birfurcation analysis in indirect field-oriented control of induction motors

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The influence of the normalized load and the rotor time constant mismatch on the dynamical behaviour of induction motors under field oriented control (IFOC) is analyzed. We focus the analysis on the Takens-Bogdanov bifurcation using a recent generalization on the Takens-Bogdanov bifurcation Theorem. Besides, we have found a criterion that allows us to determine which IFOC systems do not undergo such bifurcation.

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On an application of hybrid method to solving second ordinary differential equations

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We investigate the numerical solution of the following initial value problem

$$y'' = f(x,y), \quad y(x_0) = y_0, \quad y(x_0) = (y_0)'. \tag{1}$$

In this problem the differential equation is of special structure, i.e. the right hand side of the differential equation is solved to respect to the second derivative, and it independent of y' .

The following method is one of the effective method for numerical solution of problem (1)

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \gamma_i f_{n+i}, \tag{2}$$

and is the generalization of Stoermer's known method. If method (2) is stable, then maximal value of its accuracy equal $k+2$ that is obtained for even k (i.e. $k = 2r$). Therefore the scientists suggested different ways for constructing more precise numerical methods. One of these ways is to use the values of the second derivative of the solution of problem (1). This methods were called a second derivative multistep methods.

The scientists as Dahlquist, Enrite, Kobza, Hutya, Butcher, Ibrahimov and others have investigated this method. However, unlike the mentioned methods, here we suggest the following hybrid method

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h^2 \sum_{i=0}^{k} \beta_i f_{n+i+l_i}. \tag{3}$$

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Mathematical results for some α models of turbulence with critical and subcritical regularizations

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In this paper, we establish the existence of a unique "regular" weak solution to turbulent flows governed by a general family of α models. In particular this family contains the simplified Bradina model and the modified Leray-α model. We first consider the critical regularization for the velocity. Then, in the subcritical case, we prove the existence of weak solutions and we establish an upper bound on the Hausdorff dimension of the time singular set of those weak solutions. The result is an interpolation between the bound proved by Scheffer for the Navier-Stokes equations and the regularity result in the critical case.

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Extending the Nonsymmetric Super Time Stepping Method to Nonlinear Parabolic Equations

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We have developed an explicit super time stepping method for stiff linear systems of ordinary differential equations which have stiffness due to large imaginary eigenvalues. These systems are found in astrophysical diffusion problems, vibrational control problems, and generalized Hamiltonian systems. This method has the simplicity of an explicit method and maintains a low computational cost through the ability to maintain a reasonable time step when the imaginary eigenvalue dominates the real eigenvalue of the linear system. This conclusion is backed up by analytical and computational results. We have shown that this method also increases the computational time step size for linear problems that are only slightly nonsymmetric. Now we present preliminary analytic and computational results from applying this method to nonsymmetric nonlinear parabolic problems.

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Mathematical Modeling in Environmental Sciences and Models for Complex Media

CS-ENVIROMENT

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A Cell-Based Finite Difference Method for the Numerical Solution of PDEs

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The governing partial differential equations of fluid motion are usually numerically approximated using one of three methods: Finite Difference (FD), Finite Volume (FV) or Finite Element (FE). In this research, a new cell-centred FD (CCFD) formulation is developed that is applied in each individual cell of an arbitrary mesh discretizing the solution domain. This feature, which is motivated by development of the FV method, allows the application of the proposed FD numerical formulation on unstructured grids. As in [1], to explain this method, consider the 2D Laplace equation (1), which can be written in the discretized form (2), where second-order central differencing has been applied (see Fig. 1a for notation): $\nabla^2\phi = 0$ (1), $\frac{\phi_w - 2\phi_{cc} + \phi_e}{\Delta x^2} + \frac{\phi_n - 2\phi_{cc} + \phi_s}{\Delta y^2} = 0$ (2).

The solution procedure for node P in Fig. 1a starts by detecting all cells sharing that node. For each one of these cells: calculate the coordinates of the cell centre cc, and intersection points w, s, e and n; calculate ϕ_e by distance weighted averaging between two cc's that share e (similarly for values at w, s and n); evaluate ϕ_{cc} from eq. (2). Now ϕ_P is updated from all cc's that were detected at the beginning of this procedure. Consider the rectangular domain shown in Fig. 1b, with constant Dirichlet boundary value of 1 at the West and 0 on the other three sides. The CCFD scheme solution is shown in Fig. 1c. Comparing this result with the analytical solution of this elliptic BVP, the absolute difference averaged over all the nodes of a 25x25 grid is 0.00041. Important computational issues, such as optimum relaxation factor, accuracy, effect of grid refinement, grid clustering and associated processing times, are all investigated.

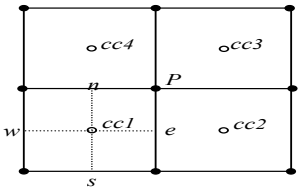
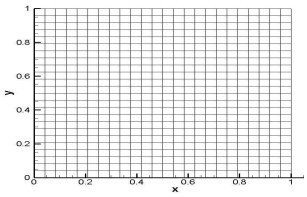
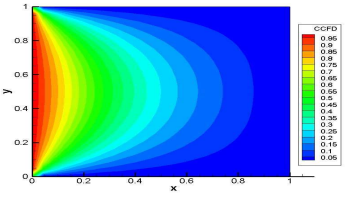


Fig. 1: (a) Cells sharing node P



(b) 25x25 grid



(c) CCFD solution

The same test case has also been solved with the CCFD scheme applied on an unstructured hybrid mesh, i.e., a combination of rectangular and triangular elements, and the results are in good agreement with the analytical solution. The CCFD scheme does not require any modification close to the boundaries, can approximate Neumann boundary conditions with the same degree of accuracy as interior nodes, and implementing higher-order differencing formulas is straightforward. A benchmark fluid flow problem has been tested with CCFD, using the vorticity-stream function formulation of the steady incompressible Navier-Stokes equation. These results will be included in the full paper.

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Time-Dynamic Modeling of Multi-Phase Flow in Volcanic Conduits

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This study models the extrusive flows and lava dome eruptions of subduction volcanoes, of which the Soufreir Hills Volcano in Montserrat is an archetype. Many factors influence the behavior of the magmatic-gas mixture in a volcanic conduit, including conduit geometry, elastic properties of the conduit walls, constitutive behavior of the magma-gas mixture, and the microlite crystallization that may accompany flow, among others. These factors can be the difference between a slow extrusion of magma and an explosive eruption. In order to understand the nature of these phenomena, we develop models of this multi-phase flow. Through our analysis, we examine changes in eruption dynamics occurring even under the assumption that conditions in the magma chamber remain constant. We approach the problem through a combination of linearized stability analysis and numerical computation. The goal of this study is to understand the principle contributions to phase dynamics and stability, specifically dealing with time dynamic solutions that address the elasticity of conduit walls.

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Effects of pressure stress work and viscous dissipation in mixed convection flow along a vertical flat plate

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The effects of pressure stress work and viscouss dissipation in mixed convection flow along a vertical flat plate are investigated. The results have been obtained by transformaing the governing boundary layer equations into a system of non-dimensional diffrential equations and by applying the implicit finite difference method together with the Newton's linearization approximation. Numerical results for different values of the viscouss dissipation parameter, the pressure stress work parameter and Prandtl number have been obtained. The velocity profiles, temperature distributions, skin friction coefficient and the rate of heat transfer have been presented graphically for the effects of the aforemensioned parameters. Results are compared with previous investigation.

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Generating space-time auto-correlated fields on the sphere

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A new approach for generating random fields on a sphere with prescribed spatio–temporal characteristics is proposed. Markov chains used as spectral coefficients generate evolving patterns on a sphere.

Random fields with prescribed spatio–temporal characteristics represent a useful tool in simulating stochastic processes, such as stochastic kinetic energy backscattering (SKEB) in ensemble weather prediction. In SKEB, the energy injected into the numerical weather prediction (NWP) model is defined by a deterministic part given by a total rate of energy dissipation involving contributions from numerical diffusion, mountain drag, and deep convection. The stochastic part, unique for each individual ensemble realization, should be represented by a reasonbly well behaved field. Not only the field must be smooth enough in space in order to allow a smooth differenciation, but also smooth enough in time in order to match time characteristics of the NWP model. At the same time, such fields must avoid the generation of unrealistically noisy patterns (from a meteorological point of view).

First order Markov chains are used to generate several sets of spectral coefficients. An expansion of spherical harmonics, as well as a Fourier expansion in the radial direction, then provide spatio-temporally auto-correlated random fields in 3+1 dimensions. Those fields on a Gaussian grid are interpolated onto the model's grid where they form, together with the dissipation function, a stream-function forcing field. The forcing field, different for each ensemble member, perturbs the velocity field of ensemble weather forecasts.

The code has been written in Fortran 90, based on object oriented programming, allowing projections on different grids. Some recent developments in spherical projection theory has been applied when writing the code.

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Heat and moisture transport system in 3D fibrous porous media with condensation/evaporation and absorption

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This paper is concerned with the heat and moisture transport in three-dimensional porous textile medium with complex phase change, condensation/evaporation and absorption. The physical process is described as a multi-phase and multi-component (air, vapor, water and heat) flow governed by a system of nonlinear, degenerate and strongly coupled parabolic equations. In this paper, we prove global existence of a weak solution under the physical assumption that the initial and background temperatures are not higher than about 1000 K.

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Financial Mathematics and Computation

CS-FINANCE

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Improved One-Factor Gaussian Copula Model for Pricing Heterogeneous Colaterallized Debt Obligations

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The one-factor Gaussian Copula model has been a market standard (Ref. [1]) for pricing Colaterallized Debt Obligations(CDOs). However, the 2007-2010 financial crisis highlighted drawbacks of this model for coping with highly correlated CDO portfolio. We introduce an improved one-factor Gaussian copula model that does not require Monte Carlo simulation. This is an extension of the pricing model proposed by Michael S. Gibson (Ref.[2]). In our improved model, instead of using flat default correlation and rate parameters across the whole portfolio, we use individual correlation coefficients between each reference entity and the market (S&P 500 index) based on 5-year daily stock prices, and we use specific rate parameter for each entity by curve-fitting the default probability term structure. Spreads from this modified model are compared to those obtained from the one-factor Gaussian copula model with flat correlation and rate parameters and the spreads' sensitivity to these parameters is also examined. Results show that uniform correlation and rate parameters fail to capture that a few or even one single asset can substantially impact the credit quality of the whole portfolio. Heterogeneity of correlations and rate parameters of different reference entities is indispensable for constructing reliable and realistic models for pricing synthetic CDOs.

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Analysis of Tax-deductible Interest Payments for Re-Advanceable Canadian Mortgages

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Our American counter-parts have been able to use their home mortgage interest costs as an income tax deductible expense. This is not the case for Canadians having a traditional mortgage. One way of transforming from non-tax deductible to tax deductible interest expenses is to borrow against home equity to make investments. The interest paid on this borrowing is tax deductible according to Canadian tax law. This can be achieved through a re-advanceable mortgage and has been promoted by personal financial planners as a way of significantly decreasing the time required to pay off a mortgage and the associated total interest cost. The promotional materials for this strategy typically make assumptions about the interest rate paid on the borrowings and the rate of return earned by the investment. What is missing from this promotional material, however, is the notion of risk associated with the investments holdings (typically a stock or mutual fund). Here we study the risk associated with this strategy to provide a better description of the mortgagor's position.

Using simulation we assess the risk to the homeowner associated with the re-advanceable mortgage. We assume that the homeowner will invest the entire proceeds from the line of credit into a single asset (e.g., stock or mutual fund) whose evolution is described by geometric Brownian motion (GBM).

We find that on average, the mortgage payoff time is less than mortgage term. However, there is considerable variation in the payoff times with a significant probability of a payoff time exceeding mortgage term. Furthermore higher the marginal tax rate, the more the average payoff time is reduced implying that this strategy is more beneficial to high-wage earners. Using a simple stochastic model for job status we also investigate the effect of job loss on the payoff time distribution.

After working with discrete time version of the evolution of stock price and the investment portfolio value, we moved to the continuous time framework. Using GBM as the evolution of stock price we were able to derive a stochastic differential equation (SDE) for investment portfolio value. Mean and variance of the distribution of investment portfolio value were derived.

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Exploiting Domain Knowledge to Forecast Heating Oil Consumption

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The GasDay laboratory at Marquette University provides forecasts of energy consumption. One such service is the Heating Oil Forecaster, a service for a heating oil or propane delivery company needing accurate forecasts of daily consumption of its customers. If a delivery service refills more often than necessary, delivery costs are higher than necessary. Accurate forecasts can reduce costs by reducing the number of trucks and drivers and by providing more efficient inventory management. If a customer runs out of fuel, the delivery service incurs costs for an emergency delivery and often a service call. Further, there is a good chance the customer will change providers. Accurate forecasts help retain valuable customers and reduce costs.

As data for each customer, we are given location, tank size, and an expert's initial estimate of consumption rate ($\mathscr{K}$-factor, gal/^{o}F). Each day, we receive a list of customers and quantities for that day's deliveries and weather reports and forecasts in the service area. We return, for each customer, estimates of oil consumption for the next 10 days. The delivery company uses our estimates to plan deliveries.

The basic modeling is simple: Fit the delivery amounts (s_k) to cumulative Heating Degree Days ($HDD_k = \sum \max(0, 60^\circ\text{F} -$ daily average temperature)), with wind adjustment, for each delivery period: $s_k \approx \widehat{s_k} = \beta_0 + \beta_1 HDD_k$, where $\beta_1 = 1/\mathscr{K}$. However, for the first few deliveries, there is not enough data to provide a reliable estimate $\mathscr{K}$, so we use Bayesian techniques with priors constructed from historical data. In practice, a delivery may not fill the oil tank because the delivery truck runs out of oil or the automatic shut-off activates prematurely. Special outlier detection and recovery based on domain knowledge is essential in this and other special cases.

A fresh model is trained for each customer with each delivery, producing daily consumption forecasts using actual and forecast weather until the next delivery. The error at each delivery is the difference between that delivery and the aggregate of daily forecasts using actual weather since the preceding delivery. Out-of-sample testing for 7/1/2009 – 6/30/2010 yields MAPE = 27.6 % and an average error of 7 % of tank capacity.

From the perspective of one one heating oil delivery company who uses this forecasting service [3], instances of one of their customers running out of oil were reduced from about 250 in 50,000 deliveries per year before contracting for our service to about 10 with our service. They delivered slightly more oil with 20 % fewer trucks and drivers, citing $250,000 annual savings in operational costs.

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Calibration of Local Volatility Models by Tikhonov-Type Regularization

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Good model selection is crucial for modern sound financial practice. A well accepted class of models consists of the local-volatility ones that were pioneered by B. Dupire in Ref. [1]. In this article we are concerned with the calibration of such models from market data. It is well known that such calibration problem, as many important ones in Finance, is highly ill-posed. In particular, small changes and noise in the data may lead to substantial changes in the results. Yet, good volatility surface calibration is crucial in a plethora of applications, including risk management, hedging, and the evaluation of exotic derivatives. In order to tackle the ill-posedness of the calibration we make use of (non quadratic) Tikhonov-type regularization techniques.

The introduction of regularization techniques in order to the stabilize the problem leads to a crucial question: If the noise in the data goes to zero, does the corresponding regularized solution converge to the true volatility? If this is the case, it would be also natural to inquire about the rate of convergence. In this contribution we analyze the continuous and discrete versions of Tikhonov regularization for the calibration of the local volatility surface and provide convergence analysis and rates for both approaches. We present a unified framework for the calibration of local volatility models that makes use of recent tools of convex regularization of ill-posed Inverse Problems. See Ref. [2,3,4].

We also consider a discrete version of the Tikhonov-type functional following Ref. [5]. Here again, we provide the convergence analysis and rates of the discrete regularized volatility with respect to the level of noise in the data and also with the discretization level, using *a priori* choice of the regularization parameter. The results are supported by numerical validations with synthetic and market data.

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Variance reduction methods for pricing and hedging exotic options beyond Black-Scholes-Merton's models

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Some drawbacks of the well known Black-Schole-Merton's model for asset prices have been verified by empirical investigations using worldwide real financial data. Therefore, more realist models (such as, exponential Levy models) for asset prices become more and more popular. However, explicit formulas for option prices usually do not exist under such more realistic models. Therefore, efficient numerical methods for option pricing and hedging are highly desirable. In this talk, we will discuss variance reduction methods combined with quasi-Monte Carlo methods for pricing and hedging some exotic options under certain exponential Levy type models. Numerical results demonstrating the advantage of the combination of variance reduction and quasi-Monte Carlo methods over the Monte Carlo method in simulating option prices and Greeks will be provided.

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A mixed integer linear programming model for optimal sovereign debt issuance

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Governments borrow funds to finance the excess of cash payments or interest payments over receipts, usually by issuing fixed income debt and index-linked debt. The goal of this work is to propose a stochastic optimization-based approach the composition of the portfolio issued over a series of government auctions for the fixed income debt, to minimize the cost of servicing debt while controlling risk and maintaining market liquidity. We show that this debt issuance problem can be modeled as a mixed integer linear programming problem with a receding horizon. The stochastic model for the interest rates is calibrated using a Kalman filter and the interest rates are represented using a recombining trinomial lattice for the purpose of scenario-based optimization. We successfully demonstrate the utility of our approach by out-of-sample back-testing on UK debt issuance data.

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A linear approximation of CVaR constraints in a multi-period portfolio selection using simulated return scenarios

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We present an extension of a single period portfolio selection model with linear approximation of conditional value-at-risk (CVaR), developed in [1], to a multi-period case. The proposed model allows one to create and maintain a multi-period portfolio with maximum return while keeping the risk under control by putting upper bounds on CVaR over all periods. This extension requires generating reliable scenarios of stock returns over the planning periods. The difficulty of generating such scenarios is due to the existence of time dependence as well as cross correlations among stock prices. Furthermore, the assumption of Gaussian distribution for daily stock returns may lead to a poor estimate of portfolio return. This issue becomes critical when the portfolio model is extended to the multi-period case. In this paper, we use an advanced synthetic data generation method for stock price scenarios using a combination of a GARCH model, Extreme Value theory, and a t-student Copula distribution based on the method in [2]. These scenarios are used for linearization of CVaR constraints and lead to a Linear Programming model.

The data set used herein includes 2600 daily prices for six stocks taken from oil and gas industry sector from yahoo finance for which the correlation coefficient matrix has also been estimated. We generated 200 scenarios for each of the stocks over 30 periods and used them for solving the multi-period optimization model. Setting an upper bound on CVaR to be $\omega = 1.7\%$ (obtained by some initial test runs) and the confidence level $\alpha = 0.95$ led to the total return of 37% at the end of final period. The multi-period model was solved several times for different values of the risk tolerance level ω. As expected, the rate of return would increase as ω was set higher. The optimization problem became infeasible for very small values of ω. On the other hand, the CVaR constraint became relaxed if ω was set too large. The return and risk of the optimal portfolio are compared against the actual return estimated by Monte Carlo Simulation. We have calculated various measures of losses for evaluating the risk of the optimal solution. Monte-Carlo simulation confirms that the same decreasing trend in mean of losses appears as seen in the optimization phase. The final return estimated by simulation is 38.5% which is slightly more than 37% obtained by optimization. CVaR constraints are violated by a small amount in 6 periods. The maximum estimated CVaR is 4.7% which is higher than 1.7% set in the optimization. This is justifiable considering the possibility of higher expected return. It would be very interesting to evaluate and compare the quality of such risk based optimal portfolios with robust portfolio solutions found in other studies. One such comparison is presented.

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Dynamic Factor Copula Model

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The Gaussian factor copula model is the market standard model for multi-name credit derivatives. Its main drawback is that factor copula models exhibit correlation smiles when calibrating against market tranche quotes. To overcome the calibration deficiency, we introduce a multi-period factor copula model by chaining one-period factor copula models. The correlation coefficients in our model are allowed to be time-dependent, and hence they are allowed to follow certain stochastic processes. Therefore, we can calibrate against market quotes more consistently. Usually, multi-period factor copula models require multi-dimensional integration, typically computed by Monte Carlo simulation, which makes calibration extremely time consuming. In our model, the portfolio loss of a completely homogeneous pool possesses theMarkov property, thus we can compute the portfolio loss distribution analytically without multi-dimensional integration. Numerical results demonstrate the efficiency and flexibility of our model to match market quotes.

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Computational Mechanics and Engineering

CS-MECHE

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Parallel FEM Simulation of Electromechanics of the Heart

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In this work, we develop a FEM model to investigate electromechanics problems [1] in the heart. The model integrates properties of cardiac electrophysiology, electro-mechanics, and mechano-electrical feedback. In order to account for large deformations of heart muscle, the updated Lagrangian approach is adopted. The parallel numerical model uses Trilinos [3] and is implemented on the supercomputer, Kraken, at the National Institute for Computational Sciences (NICS). Extensive numerical simulations are carried out on a dog ventricle to investigate the interaction of electrical and mechanical functions in the heart and their influences to cardiac arrhythmias. Fatal arrhythmias may cause sudden cardiac arrest (SCA), a leading cause of death in the industrialized world, claiming over 350,000 Americans each year [4].

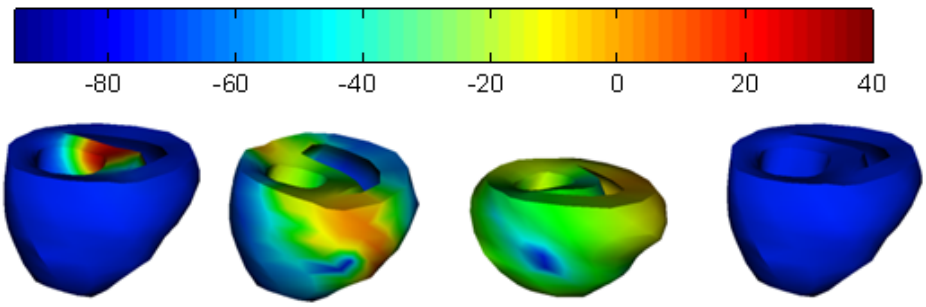

Figure 1: Mechanical deformation and electrical propagation in an impaired heart with a scar in the epicardium. The snapshots are at 1ms, 5ms, 10ms and 195ms

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Efficient Methods for Analysis of Flows in Grooved Annuli

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Annular flow passages are widely used in petroleum engineering, heat exchangers, turbomachinery, fuels cells, aero-engines and various chemical industrial devices, among many others. The flow dynamics has significant effect on the efficiency of these devices. Variations in the structure of surface topography offers potential for improving performance of flow systems in such devices. Longitudinal grooves/ribs, commonly referred as riblets, have attracted attention due to their drag reducing capabilities in turbulent flow regimes. Transverse grooves/ribs are of interest in the maximization of mixing. Effects of different forms of grooves/ribs on the pressure losses are studied in this work. Because of an uncountable number of possible shapes, an efficient method for modeling of the surface topography needs to be created as well as an efficient method for the solution of the governing equations for flows in domain bounded by grooved surfaces needs to be developed. Fourier-expansion-based representation of the surface topography is used and this provides a low-order modeling of the surface geometry. Spectrally-accurate method for solution of the field equations based on the Fourier-Chebyshev expansions is used. The irregular geometry is accounted for either (i) through the use of the immersed boundary conditions method or (ii) through the use of the domain transformation method. The former method is more efficient computationally as the main matrix remains unchanged while studying different geometries and information about geometries enters only through the boundary relations. The computational efficiency permits shape optimization of the grooves. The latter one requires reconstruction of the complete matrix for each change of geometry but is more suitable for exploration of various limits, especially flows in the presence of grooves with short wavelengths. In can be shown that the effects of the grooves may be decomposed into (i) effects due to the change in the average position of each cylinder and (ii) effects due to the shape of the grooves. The latter ones will be illustrated on the basis of extensive numerical experiments. Flow in a corrugated plane channel is recovered in the limit of large average radius of the annulus. The results show strong dependence of the pressure losses on the wave number alpha of the grooves (shape effects) and on the average radius of the annuli (global geometry effects). It is possible to achieve significant reduction of pressure losses through judicious selection of the surface topography.

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Computational Science,
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Effect of flow oscillation on dispersion of a solute in a tube

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Unsteady dispersion of a solute in an oscillatory flow is studied by using the generalized dispersion model proposed by Gill and Sankarasubramanian [1]. According to this approach the entire process is described in terms of two transport coefficients namely the convection and diffusion coefficients. In applications of our analysis to blood flows, here we modelled the flowing fluid as Casson fluid. We observed that both convection and dispersion coefficients depend on yield stress of the fluid in addition to its dependency on time. This model mainly brings out the effects of fluid oscillations and yield stress of the fluid on dispersion process. It is observed that both oscillating parameter and yield stress fluid are the strong parameters that influence the dispersion coefficients and observed both these parameters inhibits the dispersion process. This study can be used in understanding the dispersion process in cardiovascular flows.

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Effect of Biofilm Deformation on Mass transfer and Detachment forces

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Bacterial biofilms are microbes growing on surfaces and wetted interfaces in aqueous environments.They form when the cells in the fluid attach themselves to the surface and start to producing an extracellular polymeric matrix, in which the growing bacteria cells embed themselves. This gel like layer protects the embedded bacteria from harmful environmental effects such as antimicrobials and provides mechanical stability to the biofilm to resist detachment. The mechanical response of the biofilm depends not only on the material property of the biofilm but also on the shape and morphology of biofilm-flow interface. Rheology experiments done over the years by different groups on biofilms grown under different conditions using different measurement techniques have provided differing description of the biofilm response (elastic, viscoelastic solid, viscoelastic fluid) with material parameter values varying over a wide range. Most of the current mathematical models studying biofilm growth and detachment do not account for the deformation of biofilm or do so in an adhoc way to avoid numerical difficulties arising from the fluid structure interaction problem. In our work, we will present the results from our simulations where we explored how the detachment forces acting on the biofilm and the mass transfer to the biofilm are influenced by the different material descriptions used for the biofilm.

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Model and analysis of a system of a beam coupled with a rod

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This talk presents a model, analysis, and simulations of a coupled dynamic system of a thermoviscoelastic rod and a linear viscoelastic beam. It is motivated by recent developments in MEMS systems, in particular the “V-shape" electro-thermal actuator that realizes large displacement and reliable contact in MEMS switches. The model is in the form of a system of three linear partial differential equations for the beam’s and the rod’s displacements, and the temperature in the rod. The system is analyzed by setting it in an abstract form for which the existence of a weak solution is shown. Then, we present some numerical simulations of the system is, with emphasis on its vibrations.

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Numerical solution of MHD flow in a semi-infinite channel connected electrodynamically by a conductor

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The magnetohydrodynamic (MHD) flow which is laminar and steady of a viscous, incompressible and electrically conducting fluid in a semi-infinite duct under an externally applied magnetic field is considered. The flow is driven down by the current produced by a pressure gradient. The applied magnetic field is perpendicular to the semi-infinite walls which are kept at the same magnetic field value in magnitude but opposite in sign. The wall which connects the two semi-infinite walls is conducting. Thus, the coupled partial differential equations describing such flows are given in non-dimensional form as

$$\begin{aligned} \nabla^2 V + M\frac{\partial B}{\partial x} &= -1 \\ \nabla^2 B + M\frac{\partial V}{\partial x} &= 0 \end{aligned} \qquad \text{in } \Omega$$

where Ω is the upper semi-infinite duct, $\{(x,y)\,|\,-a \le x \le a,\, y \ge 0\}$, and M is the Hartmann number. $V(x,y)$ and $B(x,y)$ are the dimensionless velocity and the induced magnetic field, respectively. The boundary conditions which are suitable in practice for the MHD flow in an infinite region can be expressed as

$$\begin{aligned} V(\pm a, y) &= 0 && 0 \le y < \infty \\ V(x,0) &= 0 && -a < x < a \\ B(\pm a, y) &= \pm k && 0 \le y < \infty \\ \partial B/\partial y(x,0) &= 0 && -a \le x \le a \end{aligned}$$

where the conductivity changes abrubtly at the discontinuity points $(\pm a, 0)$. Moreover, the velocity, V, magnetic field, B, and their normal derivatives satisfy the regularity conditions as $y \to \infty$.

A boundary element method (BEM) solution is obtained by using a fundamental solution which enables to threat the MHD equations in coupled form with general wall conductivities. The inhomogeneity in the equations due to the pressure gradient is tackled obtaining a particular solution, and the BEM is applied with a fundamental solution of coupled homogeneous convection-diffusion type partial differential equations. Constant elements are used for the discretization of the boundaries ($y = 0$, $-a \le x \le a$) and semi-infinite walls at $x = \pm a$ by keeping them as finite, since the boundary integral equations are restricted to these boundaries due to the regularity conditions as $y \to \infty$. Numerical calculations are carried out for moderate values of Hartmann number ($M \le 50$) with several values of boundary conditions for the magnetic field, k, on the non-conducting walls. The results are presented in terms of equi-velocity and magnetic field contours which show the effect of M and k on the flow behaviour. It is noted that the velocity becomes uniform at the center of the duct with an increase in M, and thus the flow becomes stagnant. In addition, as M increases the boundary layer formation starts taking place on the non-conducting boundaries for both the velocity and the magnetic field.

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Numerical Bifurcation Study of Natural Convection in a Layer of Fluid Subject to Spatially Distributed Heating

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We present the numerical investigation of the Navier-Stokes equations for the problem of Rayleigh-Benard convection (RBC) in a slot whose bottom wall is subject to a long-wavelength heating and the upper wall is isothermal. Due to nonlinearity of the equations and a large number of possible bifurcations, RBC has been one of the well-known classical hydrodynamic stability problems and attracted lots of efforts during the past century. In this work, the bifurcation process as a function of the pattern of spatial distribution of the heating (as measured by the heating wave number α) and the amplitude of the heating (as measured by the relevant Rayleigh number Ra) for two distinct fluids (as specified by Prandtl number Pr) have been investigated. Two types of bifurcations, i.e. pitch-fork bifurcation and "bifurcation from infinity", have been identified depending on the wave number of the heating and heating intensity. A continuous "fan" of bifurcation branches emanating from the same bifurcation point has been found in some cases.

Since in a numerical simulation there is some uncertainty about the accuracy of the results, we have carried out solution using different computational methods in order to ascertain the validity of the results. Three numerical techniques, including Spectral Chebyshev-Collocation, Variable-Step-Size Finite-Difference, and Finite-Volume Methods have been used to solve the governing equations. Results produced by these methods identify the same characteristics of convection in the zone where multiplicity of solutions exists. Besides, an asymptotic solution has been developed for the limit $\alpha \to 0$; its testing demonstrated good consistency with the numerical results. Multiple flow structures associated with the same conditions can be produced by changing the history of the heating; this history can be controlled by using different initialization conditions, different continuation strategies in the parameters space as well as by using different solvers.

It was observed that convection has a simple topology consisting of one pair of counter-rotating rolls per heating period when the Rayleigh number Ra does not exceed the critical value of 427. Secondary motions in the form of rolls aligned in the direction of the primary rolls and concentrated around the hot spots occur for supercritical values of Ra. When heating intensity is sufficiently small but larger than the critical value, i.e., $427 < Ra < 470$, the secondary motions correspond to supercritical pitchfork bifurcations and occur only if α is sufficiently small, i.e., $\alpha < 0.14$. Increase of heating intensity to $Ra > 470$ results in secondary motions occurring at larger values of α, i.e. $\alpha > 0.14$, and bifurcation changing character into "bifurcations from infinity". Changes in the form of secondary motions have been traced by constructing bifurcations diagrams in the (α, Nu_L) plane for fixed values of Ra, and in the (Ra, Nu_L) plane for fixed values of α, and thus permit creation of a global diagram in the (α, Ra, Nu_L) space. Here Nu_L is the local Nusselt number calculated over the hot spot. Processes described by these diagrams are insensitive to variations of the Prandtl number for $Pr = 0(1)$ as only small differences have been observed between results for $Pr = 0.7$ and $Pr = 7$. This work complements the previous investigations on this subject by extending the analysis of heating patterns toward small and very small wave numbers ($0.01 < \alpha < 0.5$). This is the first time, to the best of our knowledge, that the effects of such patterns have been discussed and the corresponding bifurcation processes have been analyzed.

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Large-Eddy Simulation of Streamwise Rotating Turbulent Thermal Channel Flows Based on Dynamic Nonlinear Subgrid-Scale Models

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Numerical simulation of rotating turbulent thermal flows represents a challenging topic with important applications in rotary machinery, turbo-machinery and rotating heat exchangers. In response to the Coriolis and centrifugal forces, large secondary flows are induced in rotating flows, which then dramatically alter the flow structures and the process of heat and mass transfer. As a consequence, the physical mechanisms underlying the transport of momentum, heat and mass in rotating flows are subject to further dynamical complexities, which impose additional challenges on the predictive accuracy of turbulence models. Over the past decades, extensive research has been conducted experimentally and numerically in order to understand the physics of rotating channel flows. However, most of the previous studies have focused on heat and fluid flows subjected to spanwise rotations.

In large-eddy simulations (LES) of rotating thermal channel flows, the filtered continuity, momentum and thermal energy transport equations together form the system of governing equations for determining the filtered velocity and temperature fields. As a consequence of the filtering process, the so-called subgrid scale (SGS) stress tensor and SGS heat-flux (HF) vector appear in the filtered momentum and thermal energy equations, which need to be modeled in order to close the system of governing equations. To date, the dynamic nonlinear model (DNM) of Wang and Bergstorm [1] for modelling the SGS stress tensor and the dynamic full linear tensor thermal diffusivity model (DFLTDM) of Wang *et al.* [2] for modelling the SGS HF vector, have only been tested using a few canonical test cases such as Couette and Poiseuille flows, and mixed natural and forced convection in horizontal and vertical channels. In contrast to the previous studies, the present research aims at examining the predictive performance of these two advanced dynamic SGS models in the context of heated channel flows subjected to streamwise system rotations. In order to examine the effects of rotation on the heat and fluid flows, different rotation numbers (defined using the angular velocity of the rotating channel and the wall friction velocity) ranging from 0 to 15 were tested. The predicted LES results on the first- and second-order statistics of the resolved velocity and temperature fields are compared with a comprehensive DNS data set in order validate the proposed numerical approach.

In the final paper, more detailed analysis of the flow characteristics will be presented, including, e.g. the budget of the shear stresses and heat fluxes, Reynolds number effects, and forward and backward scatter of SGS kinetic energy between the resolved and unresolved scales. Furthermore, the heat transfer effects in conjunction with the turbulent flow field under the influence of the Coriolis and centrifugal forces will also be thoroughly analyzed.

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Partial Differential and Integral Equations in Mathematical Modeling

CS-MODELING

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The use of the Fourier transform for solving linear elasticity problems

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This paper deals with solving linear elasticity problems using a fictitious domain method and an effective solver based on the Discrete Fourier transform and the Schur complement reduction in combination with the null space method. The main goal is to show step by step of solving elliptic boundary value problems for linear elasticity using above mentioned methods. We consider elastic body represented by domain $\omega \subset R^2$ with boundary $\gamma = \overline{\gamma_u} \cup \overline{\gamma_p}$. The zero displacement is imposed on γ_u while surface tractions of density $p \in (L^2(\gamma_p))^2$ on γ_p. Let us formulate linear elasticity problem:

$$\left.\begin{array}{rcll} -div\,\sigma(u) & = & f & \text{in } \omega, \\ u & = & 0 & \text{on } \gamma_u, \\ \sigma(u)\nu & = & p & \text{on } \gamma_p, \end{array}\right\}$$

where $\sigma(u)$ is the stress tensor in ω and ν is the unit outward normal vector to γ. We prescribe forces of density $f|_\omega \in (L^2_{loc}(R^2))^2$ in ω. The stress tensor is related to the linearized strain tensor $\varepsilon(u) := 1/2(\nabla u + \nabla^T u)$ by Hooke's law for linear isotropic materials $\sigma(u) := \lambda\, tr(\varepsilon(u))I + 2\mu\,\varepsilon(u)$ in ω, where "tr" denotes the trace of a matrix, $I \in R^{2\times 2}$ is the identity matrix and $\lambda, \mu > 0$ are the Lamè constants.

We start from the fictitious domain formulation of a given problem. The main idea of this method is to embed a real domain ω of the original problem with possibly complicated geometry to a new simple shaped domain Ω called fictitious domain. The original problem is reformulated to a new one defined in the fictitious domain Ω. The advantage is in using special partition on Ω, which enable us to apply effective solvers to compute the solution of resulting algebraic system. We consider the original boundary conditions as a constraint which we enforce by Lagrange multipliers defined on the boundary γ of the original domain ω, therefore solution has a singularity on γ. We propose a new approach in which we move singularity away from boundary γ to get smoother solution (Ref.[1]).

The discretization of fictitious domain formulation of equation 1 using finite element method leads to the algebraic saddle-point system, where the stiffness matrix A appears. Due to the choice of the space with solution with periodic boundary condition on $\partial\Omega$, the matrix A is singular, but the advantage is that A has a block circulant structure which allows to use highly efficient solver based on the Fourier transform (Ref.[2]). We use spectral decomposition of matrix A to evaluate $A^\dagger y$ by Fast Fourier Transform without storing A and it is big advantage against other algebraic solvers. Here $A^\dagger$ is the generalized inverse which arises after applying the Schur complement reduction and the null space method for solving this problem.

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Inverse scattering problems for the Hartree equation whose interaction potential decays rapidly

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We consider the inverse scattering problem for the three-dimensional Hartree eqation

$$i\partial_t u + \Delta u = (V * |u|^2)u, \quad (t,x) \in \mathbf{R} \times \mathbf{R}^3. \tag{1}$$

Here, $u = u(t,x)$ is a complex-valued unknown function, $i = \sqrt{-1}$, $\partial_t = \partial/\partial t$, $\Delta = \partial_1^2 + \partial_2^2 + \partial_3^2$, $\partial_j = \partial/\partial x_j$ $(j = 1,2,3)$, $V = V(x)$ is a real-valued measurable function, the symbol $*$ denotes the convolution in $\mathbf{R}^3_x$. The equation (1) is approximately derived by the time-depedent multi-body Schrödinger equation and the function $V(x)$ means the interaction potential for particles. It is well-known that if $V \in L^p$ for some $1 \leq p \leq 3/2$, then the scattering operator S for (1) is well-defined on some 0-neighbourhood in the Sobolev space H^1.

The inverse scattering problem for the perturbed Schrödinger equation is to recover the perturbed term by applying the knowledge of scattering operator S. By [2], we see that if $V \in L^1$, then the value of $\mathscr{F}V(0)$ can be determined by the following formula:

$$\mathscr{F}V(0) = \frac{\lim_{\lambda \to 0} \lambda^5 I[\phi_\lambda]}{(2\pi)^{3/2} \|e^{it\Delta}\phi\|^4_{L^4L^4}}, \quad \phi \in \mathscr{S} \setminus \{0\}.$$

Here, $\mathscr{F}V$ is the Fourier transform of V, $\phi_\lambda(x) = \phi(\lambda x)$ and

$$I[\phi] = \lim_{\varepsilon \to 0} \varepsilon^{-3} \langle S(\varepsilon\phi) - \varepsilon\phi, \phi \rangle_{L^2}$$

By [1], we see that if V is radial and satisfies

$$\int_{\mathbf{R}^3} e^{\alpha|x|} V(x) dx < \infty$$

for some $\alpha > 0$, we can determine the value of $\partial_\rho^m \nu(0)$ for any non-negative integer m. Here, $\nu(\rho) = \mathscr{F}_{r \to \rho} V_0(\rho)$, $V_0(r) = V(x)$ $(r = |x|)$.

In this talk, we show if $V(x)$, which may be non-radial, satisfies (2), then we can determine the value of $\partial_\xi^\beta \mathscr{F}V(0)$ for any multi-index β.

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Domain decomposition strategies with black box subdomain solvers

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Most domain decomposition methods imply the repeated solution of subdomain problems, that do actually constitute the bulk of the computation. Since extremely efficient optimized monodomain solvers for a wide range of problems are already implemented and available in commercial/academic codes, it is desirable to have the possibility of using such solvers directly in the solution process, and to have a solution strategy in which the subdomain solving step can be performed by entirely relying on such codes as they are, without need of modifying them or even of handling them in ways which have not been foreseen and documented by the programmers. Though many non conforming domain decomposition methods allow in principle to use independent subdomain solvers, most of the times the coupling condition implies some modification for the corresponding code (al least in terms of input and/or output). In particular the standard non conforming domain decomposition strategies involve the solution of Dirichlet problem and demand the subdomain solvers to provide the outer normal derivative of the solution as output data. This kind of output data is not always implemented in PDE solvers and this limits the use of many commercial/academic codes in the framework here considered. In order to overcome this limitation we propose and test here a domain decomposition strategy based on a continuous version of the FETI method ([2][3], which will allow, at the discrete level, to treat the subdomain solver step as a simple standard call to monodomain codes, without the need for such codes to provide any output information on the outer normal derivative of the solution, the minimal requirement on the code being the ability to solve problems with mixed Dirichlet/Neumann boundary conditions.

Stability and accuracy of the resulting domain decomposition method will be discussed under quite general assumptions on the subdomain solvers ([1]), and tests of the method proposed will be performed with the *MATLAB©PDE Toolbox* in two dimensions and with *COMSOL©* in three dimensions.

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Wavelet Analysis of Solitons and its Energy aspect

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In mathematics and Physics, a soliton is a self re-inforcing solitary wave (or a wavelet packet or a pulse) that maimtains its shapewhile it travels at a constant speed. Solitons arise as the solutions of a widespread class of weakly non-linear dispersive ODE, PDE- describing physical systems- including Non-linear Schrodinger Equation (NLS), Kortenez-de Vries equation (KdV),mSine-Gordon equation(S-G). The soliton solutions are typically obtained by meas of inverse scattering transform and owe their stability to the integrability of field equations. The mathematical theory of these equations is a broad and very active field of research. Wavelet theory is the mathematics associated with building a model for a signal, system or process with a set of special signals. The connections with research in other fields have emerged and become clarified in recent years. In this paper, first part deals with establishing a strong relationship of Wavelet transform with Fractional Fourier Transform (FrFT) in n-dimensional set up and by exploiting this relationship, WT is extended to the spaces of Tempered Distributions. In this theoretical framework, a Wavelet transform which makes use of envelop soliton solutions as its Analysing Wavelet (AW) is proposed in the second part. Suitability of this transform for analysing solitons in this system is discussed. In the end, tha characterisation for Energy distribution in this Wavelet representation of solitons is obtained

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Dynamic models for the Gao beam

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We present recent results on the modeling, analysis, and simulations of the dynamics of systems that contain a nonlinear Gao beam. The interest in the beam lies in that it exhibits vibrations about buckled states. We present the models, and some recent theoretical existence and uniqueness results. Then, we discuss contact problems for the beam, either with a reactive foundation, or with two stops. Also, we shortly describe the use of the beam in MEMS systems. The simulations show interesting types of vibrations about a buckled state and the related noise.

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Dynamic model for the Gao beam - Regularity and Contact

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The talk describes the Gao beam model for a nonlinear beam that exhibits vibrations about a buckled state. The model is presented and its analysis summarized. In particular a higher regularity of the weak solution is obtained. Then, the process of dynamic contact between the beam and a rigid or reactive foundation is described and analyzed. The contact is modeled with the normal compliance condition for the deformable foundation, and with the Signorini condition for the rigid foundation.

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Shock−turbulence interaction: details of a classifying construction

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A model of shock-turbulence interaction is constructed in presence of a *minimal* nonlinearity. We consider a *linearized* (with shock) context: which consists in a *linear* problem with a *nonlinear* subconscious. A nonlinear subconscious results when the nonlinearity is allowed only at the zeroth order of a perturbation expansion: a piecewise constant admissible solution [with shock; zeroth order] is perturbed; one linearizes and proves that the zeroth order requirement of admissibility is still active at the first order and essentially structures the linearized description. Consequently, the interaction solution is essentially constructed as an admissible [entropy] solution.

The incident turbulence is considered to have a *vorticity* nature and is modelled, using the *linearized* context, by a non-statistical/noncorrelative *superposition* of some finite (or point core) planar vortices.

The present analysis has essentially two objectives: (*a*) finding an *analytic, closed, optimal, highly nontrivial* form for the interaction solution, and (*b*) offering a *classifying characterization* of this interaction solution.

Realizing the objective (*a*) is connected with:

- considering a *singular limit* of the interaction solution,
- considering a *hierarchy of (natural) partitions* of the singular limit,
- inserting some (natural) *gasdynamic factorizations* at a certain level of the mentioned hierarchy and
- noticing a *compatibility* of these factorizations (indicating a gasdynamic *inner coherence*),
- *predicting some exact details* of the interaction solution,
- indicating some parasite singularities [= strictly depending on the method] to be compensated [= pseudosingularities],
- *re-weighting*the singular limit of the interaction solution into an analytic, closed, optimal, highly nontrivial form.

Realizing the objective (*b*) is connected with finding some *Lorentz arguments of criticity*. The interaction solution appears essentially to include a *subcritical* and, respectively, a *supercritical* contribution distinguished by differences of a *"pseudo relativistic"* nature. Precisely: in the singular limit of the interaction solution the emergent sound is *singular* in the subcritical contribution and it is *regular* in the supercritical contribution.

- The structure of the present interaction solution is associated first, from a classifying prospect, to the Lighthill fundamental paper where the incident turbulence is acoustically modelled by a distribution of quadrupoles − which is equivalent with a weighted distribution of point vortices.
- The present interaction solution parallels and extends, from an analytical prospect, the Ribner representation and computational approach corresponding to the interaction between a shock discontinuity and a planar vortex whose axis is *parallel* to this discontinuity.
- The details of the "pseudo relativistic" separation inside the constructed interaction solution are finally compared with the criticity arguments considered in the recent fundamental numerical studies on the shock-turbulence interaction due to S.K. Lele or K. Mahesh, S.K. Lele and P. Moin.

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The motion of a gao beam between two stops

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Elastic or viscoelastic (Kelvin-Voigt type) beams that we have considered in the dynamic contact problems are mostly linear beams such as EulerBernoulli beams or Timoshenko beams. However, we study dynamic contact of a nonlinear beam which is developed by Gao [2] in 1996. We assume that its left end is rigidly attached and its right end is constrained to move between two rigid stops. Thus, Signorini contact conditions which can be interpreted in terms of complementarity conditions are imposed on the right end of the beam. The similar dynamic contact model has been previously studied by two papers; one paper [3] is about vibrations of a viscoelastic Euler-Bernoulli beam and the other one [1] is about vibrations of a viscoelastic Gao beam. We note that the left end of Gao beam is clamped in the paper [1]. In addition, numerical schemes were not presented in those papers. In this work, we will not only prove the existence of solutions but also compute numerical solutions. Our numerical schemes are to use the time discretization over the time interval and Galerkin approximation over the spacial domain. Furthermore, the next time step solution that arises in the nonlinear system will be solved by fixed point iteration. One of our major concerns is to investigate energy balance which will be shown theoretically and will be supported numerically.

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Computational Science,
Waterloo, Canada, July 25-29

Wave−wave interactions of a gasdynamic type

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Two gasdynamic analytic approaches [of a Burnat type / Martin type] are respectively used in order to construct two analogous and significant pairs of classes of solutions [isentropic pair / anisentropic pair]. Each mentioned pair puts together a class of "wave elements" and a class of "wave-wave regular interaction elements". A classifying parallel is finally constructed between the two analogous pairs of classes – making evidence of some consonances and, concurrently, of some nontrivial contrasts.

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On conformal mappings of spherical domains

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The problem of the generation of uniform mappings for spherical domains is one of the oldest problems of cartography and geodesy as well as the important part of developing efficient numerical schemes for geophysical modeling, in particular, for atmosphere-ocean dynamics. In cartography, one of the central problem is developing the planar representations of the Earth surface with the minimum possible distortion for the chosen class of mappings. In modeling large-scale atmosphere-ocean processes, approximate solutions of the governing nonlinear partial differential equations are found by applying numerical methods that requires generation of computational grids over spherical domains with the most possible uniformity in order to produce more accurate and efficient numerical algorithms.

Conformal mappings are one of the most used tools for planar representation of the sphere surface in cartography and geophysical sciences. Each conformal mapping can be characterized by its scale function representing the ratio between spherical and planar elementary arc lengths. In this study we consider the problems of restoration of the conformal mapping starting from a given scale function and construction of the most uniform projections for spherical domains using the Chebyshev criterion of the optimality. Both problems can be formulated as finding the solutions to the system of partial differential equations including the Cauchy-Riemann equations (the conformality conditions), the nonlinear cartography equation (the restoring condition) and the Laplace-Beltrami equation for scale function (the condition of the spherical curvature). The optimality problem requires constant boundary conditions for the last equation. We solve the restoration problem for arbitrary spherical domain in the class of conformal mappings with a scale function depending only on latitude. The obtained mappings are compared with the traditionally used Riemann, Lambert and Mercator conformal projections. The uniformity level of the optimal conformal mappings is compared with that of the selected orthogonal projections.

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On a class of non-linear elliptic over-determined problems in a doubly connected domain

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We deal with a class of non-linear over-determined elliptic problem in a doubly connected domain. Based on P-function and classical formula of Green, we show that the solution is radially symmetric and the domain in consideration is an annulus of N concentric spheres. Our approach does not recourse to the maximum principles nor to the moving plane.

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Modelling Magnetic Field Profiles near Surface of Rough Boundary Superconductors

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Recent low energy experiments on superconductors show that shielding currents near the surface appear to be suppressed. One possible explanation is that of surface roughness. In our modelling, we took a sinusoidally varying surface and applied asymptotic analysis and finite difference discretizations to analyze the field behaviour near the surface. Our results offer insights into the effects of surface roughness: we discover new small-scale behaviours that have not yet been detected in experiments, and we demonstrate that within the model we used, that surface roughness alone cannot explain the experimental results.

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A second order time scheme for the Landau-Lifshitz-Gilbert equation

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Micromagnetism is a continuum theory for modeling ferromagnetic materials. The magnetization of a ferromagnetic system Ω is a vector field $m : \Omega \in \mathbf{R}^3 \to S^2$ that obeys the Landau-Lifshitz-Gilbert equation:

$$\alpha \dot{m} - m \times \dot{m} = H - \lambda m \tag{1}$$

with the Brown condition $\partial m/\partial n = 0$ on the free surface $\partial\Omega$. Contributions to the effective magnetic field $H(m)$ are the exchange field Δm, the demagnetizing field $H_d(m)$ and possibly others, $\lambda(m)$ stands for $H(m) \cdot m$ and α is a phenomenological damping constant.

With a time discretization of step k, and $m^n = m(t^n)$ being given, the main question is how to apply the constraint $m^{n+1} \in S^2$. The strategy is to find an approximation v to $(m(t^n + k) - m^n)/k$, then set m^{n+1} as the projection of $m + kv$ onto S^2. The test space adapted to the problem, introduced by Alouges [1], is the tangent plane to m that is $T = \{w \in H^1(\Omega, R^3),\ w(r) \cdot m(r) = 0\ a.e.\}$. It is then possible to write a well-posed formulation for the explicit scheme as well as inconditionally stable schemes of first order. The difficulty in achieving a second order scheme is the projection on S^2.

We show that a second order scheme is achieved by projecting a midpoint rule on the tangent plane and that the scheme is stable using a theorem of Bartels' [2]. A fixed-point iteration is used for the resolution. The costly part is an additional computation of demagnetizing field; for this purpose we use fast summation methods like the FMM (Fast Multipole Method) and the NFFT (Non-uniform Fast Fourier Transform).

The second order scheme was implemented in our micromagnetic code named FELLGOOD. Results obtained on the fourth standard problem of the NIST [3] – nonlinear dynamics on a Permalloy platelet, are very close to those of Finite Volume codes. Compared to the first order scheme, the new scheme allows to gain a factor ≈ 10 in computation time.

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Evaluating the effect of implementing biologically realistic delays on hepatitis C kinetics and associated estimates of antiviral efficacy

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Hepatitis C is an infectious disease caused by the hepatitis C virus (HCV). In the majority of cases, infection by HCV causes chronic disease and in some cases hepatocellular carcinoma. No vaccine is available for HCV and current therapy with interferon-α (IFN-α) is effective in controlling the infection in less than half of treated persons. The absence of a reliable in vitro cell culture model for HCV has limited the quantitative specification of the HCV infection dynamics. However, mathematical models have had some success in describing the dynamics of HCV during antiviral treatment of patients.

Current mathematical models of the HCV infection are based on a set of ordinary differential equations (ODEs) which have had success both in representing the qualitative features of the observed virus decay under treatment and have allowed for the determination of antiviral efficacy and other important parameters of the viral infection process [1]. Despite this success, some of the underlying assumptions in these models may not be biologically realistic. For example, these models assume that upon infection a cell immediately begins producing and releasing new virions. Also, the use of ODEs implies an assumption that the distribution of transition delays between stages of cellular infection are exponential.

Here, we consider a more biologically realistic mathematical model and implement it to describe the dynamics of HCV under antiviral therapy. This model includes an "eclipse" phase between the moment of a cell's infection and the release of new virus. In addition, the model allows for arbitrary distributions of delays between infection stages. The use of normal and log-normal delays, for example, enforce a minimum waiting period before a cell transitions from one state to another. Application of the new model to viral titer data for patients undergoing antiviral therapy leads to different conclusions about the efficacy of the antivirals.

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Characterizing the efficacy of combination antiviral therapy for the treatment of influenza

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Influenza is a serious disease that can circulate worldwide, affect people of any age, and cause severe illness and death. Since a vaccine takes at least six months to develop from the time a new influenza strain is identified, antiviral drugs are the first line of defense against a novel flu strain. There are two major classes of anti-influenza drugs, adamantanes (M2 channel inhibitors like amantadine and rimantadine) and neuraminidase inhibitors (such as oseltamivir and zanamivir). Antivirals are highly effective but resistance against them has risen to high levels, rendering them often ineffective.Combination therapy is showing promise in increasing antiviral effectiveness [1], but determining the optimal antiviral dose combination experimentally is complex and costly.

Our aim is to use mathematical models of influenza infections to simulate combination therapy. We analyze the dynamics of influenza viral infections in Madin-Darby Canine Kidney cells inside a hollow-fiber in the presence of constant concentrations of amantadine or oseltamivir to determine the best model for representing the effect of these drugs. The results of this analysis are used to construct a model that can simulate combination therapy. This model is used to determine the synergistic or antagonistic effect of combining the two drugs and can be used to guide clinicians in determining the optimal doses for use in combination therapy.

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Molecular Dynamics Simulations Indicate that Prothymosin Alpha and Nrf2 Bind to Keap1 via Preformed Structural Elements and Coupled Folding and Binding

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Intrinsically disordered proteins (IDPs) are abundant in cells and have central roles in protein-protein interaction (PPI) networks. Interaction between the intrinsically disordered Prothymosin alpha (ProTα) and the Neh2 domain of Nrf2, with a common binding partner, Keap1, is an important PPI for regulating cellular response to oxidative stress. Misregulation of this pathway can lead to neurodegenerative diseases, premature aging and cancer. Crystal structures of ProTα and Neh2 peptides in complex with the Keap1 reveal that they occupy the same site on the Kelch domain of Keap1 and adopt similar bound-stateβ-turn conformations. In order to understand the mechanisms these two disordered proteins employ to bind to Keap1, molecular dynamics (MD) simulations were used to study the structure and dynamics ofProTα and Neh2. Our results show that in their free states, both ProTα and Neh2 have propensities to form bound-state-like β-turn structures but to different extents. Specifically, the Keap1-binding region of Neh2 samples β-turn conformations with lower RMSD to its bound state structure and with higher frequency. Hydrogen-bond analysis suggests this is the result of a greater number and more frequent intra-turn hydrogen bond formations in the free-state of Neh2. We also found that, for both proteins, residues outside the Keap1-binding motifs may play important roles in stabilizing the bound-state-like structures. Based on the results, we propose that the binding of disordered ProTα and Neh2 to Keap1 occurs synergistically via preformed structural elements (PSEs) and coupled folding and binding, with a heavy bias towards PSEs, particularly for Neh2. Our results provide insights into the molecular mechanisms Neh2 and ProTα bind to Keap1, information that is useful in developing therapeutics to enhance the oxidative stress response.

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Modelling time-dependent drug concentrations with constant drug concentration in within-host models of influenza

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When studying drug effects in models of human disease, drug concentration is often assumed to be constant. This is unrealistic as drugs are often taken as pills at discrete times. The drug concentration at the target site increases upon ingestion of the pill and then decays as the drug is metabolized by the body. Thus, the typical drug treatment profile varies with time. We aim to determine whether this type of impulsive drug concentration can be modelled by a constant drug concentration.

We use a pharmacokinetic model to generate a realistic time varying drug concentration. We apply the varying drug in a viral kinetics model to generate a viral titer curve. Least-square fits are then used to find a constant drug concentration and treatment delay that reproduce the viral titer. Using this method, we determine the relationship between the impulsive drug concentration and the constant drug concentration. Determining this relationship permits us to convert an impulsive dose to a constant drug concentration and justifies the simplifying assumption of constant drug concentration in within-host models of influenza.

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Studying the quality of noise in a large biochemical reaction network as a function of the system volume

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Mathematical and statistical modeling play an essential role in the study of random fluctuations in biochemical systems. Chemical reactions are stochastic in nature and the time-evolution of biochemical processes can be described rigorously only by means of a probabilistic approach. Based on the theory of stochastic chemical kinetics, a continuous-time discrete-state Markov model for a reacting system can be formed [1]. The Markov model is described by the so-called chemical master equation (CME). In simulation studies, the CME is typically simulated using the Gillespie stochastic simulation algorithm (SSA) [1].

The stochastic modeling approach is essential especially when small intracellular systems are studied [2]. To be able to develop better models for intracellular signaling and to understand the role of biochemical noise more throughly, the quality of noise must be studied in a quantitative manner. Analytical results regarding the quality of noise might be attainable for some simple systems but in general such results are out of reach. Biochemical systems are often large and complex, include strong nonlinearities, and the system behavior as well as the quality of noise can be studied only through simulations.

In this study, we implement a large nonlinear signal transduction network combining protein kinase C, mitogen-activated protein kinase, phospholipase A2, and β isoform of phospholipase C networks. We simulate the network in 300 different cellular volumes using the Gillespie SSA and study how the quality of noise changes as a function of volume. We analyze the simulation results by computing statistical characteristics of the realizations as well as by approximating the frequency domain behavior using Fourier methods. In the implementation, we use modern parallel computing techniques which enable us to perform simulations in a reasonable time.

We conclude that basic frequency domain techniques such as the numerical Fourier analysis can be applied to the analysis of simulation results produced by the Gillespie SSA. This approach is suited not only to the study of fluctuations but also to the study of pure noise processes. Noise seems to have an important role in biochemical systems and its properties can be numerically studied by simulating the reacting system in different cellular volumes. Accurate statistics can be obtained from computational studies by using parallel computing techniques which make it possible to run massive simulations. Our simulation results show how the noise strength depends on the volume and indicate that there are several kinds of noise processes in the network. A common feature for all of the studied noise processes is a spectrum having a shape that can be described by a power law.

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Investigating the impact of cell tropism on influenza infection spread in computer-simulated lung tissue

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The severity of influenza virus infections in humans may depend on the properties of the cells which are infected. There are two main types of cells in the human lung that are targeted by the virus, which possess two types of receptors which mediate entry of virus into the cell: non-ciliated cells characterized by α-2,6 receptors, and ciliated cells characterized by α-2,3 receptors [1]. Non-ciliated cells are predominantly distributed in the upper airway and are more readily infected with human influenza strains, whereas ciliated cells are more readily infected by avian (bird-derived) influenza strains. In previous work, an ordinary differential equation (ODE) model was implemented to study the dynamics of an infection with two available target cell types. This two-cell model was the first mathematical model explaining the sustained high viral titers characteristic to avian influenza infections in humans.ODE models however, do not incorporate any spatial effects which may be important in the geometry of the respiratory tract.

We implement an agent based computational model that can simulate in-host influenza infections with two target cells and predict their outcomes. This model treats host cells as discrete units and assigns stochastic dynamics for each within a set of preset parameters. Spatial distribution of cell types is incorporated as a gradient across the computational grid.

We explore the effects that spatial considerations have on an influenza infection, with a particular focus on understanding the connections between infection severity and the location of the infection within the respiratory tract.

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Faster Short DNA Sequence Alignment with Parallel BWA

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Variations in the genomes of individuals have been found to be responsible for a large degree of human diver- sity such as physical appearance and susceptibility to disease. Therefore, identification of such genetic variations has important implications in biological and medical genetic research. Newly available technologies enable the generation of DNA sequences at billions of relatively short DNA sequence reads and sequencing of a large number of genomes relatively quickly. These sequences can be used to identify genetic variations by first aligning with a reference genome sequence, using computer algorithms that make use of approximate string matching and string indexing methods. The process of aligning a very large number of short sequence reads generated by next-generation sequencing (NGS) technologies is very computationally intensive, and this has led to the development of many sequence mapping programs. While new software such as BWA[1], SOAP2[2], and Bowtie[3] are able to efficiently align large numbers of short DNA sequences, we proposed that parallel computing would aid in providing additional speedup in data processing. For this purpose, we have developed pBWA, an efficient parallel version of BWA, a popular NGS alignment tool, using the OpenMPI library on the SHARCNET[4]. pBWA retains and improves upon the multithreading provided by BWA while adding efficient parallelization for the original core alignment functions. Initial tests have been performed on SHARCNET's Orca cluster by aligning 350 million 50 bp SOLiD reads to the mouse genome. This test took 25 hours to complete using the original multithreaded BWA with 24 threads, while the same task was completed in just over 2 hours using 240 processors with pBWA, reaching about twelve-fold speedup in wall-time. When combining multithreading with pBWA, over forty-fold wall-time speedup has been witnessed. pBWA has shown that its wall-time speedup is bounded only by the size of the parallel system. This is due to the fact that pBWA can simultaneously utilize any number of nodes, unlike multithreaded BWA which can only run on as many cores as a single node possesses. The availability of pBWA is expected to facilitate NGS data analysis via use of high performance computing.

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Molecular Dynamics Studies of Transportan Interacting with DPPC Lipid Bilayer

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Translocation of peptides through cellular membranes is a fundamental problem in developing antimicrobial peptides and also in drug delivery. It is known from experiments that there are a number of very different classes of peptides, all known as cell-penetrating peptides, that are able to penetrate membranes and, for example, carry pharmacological compounds-thus a promising strategy for drug delivery. It is not known, however, what are the physical mechanisms that facilitate the translocation. We performed a series of molecular dynamics simulations to study the nature of interactions between one of these peptides, namely Transportan, and a zwitterionic DPPC bilayer. Our objective is to find the controlling mechanisms of translocation through a detailed analysis of peptide-lipid interactions and free energy analysis.

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To estimates of the solutions and the free boundary for one nonlinear heat conductivity equation

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Consider in the domain $Q = \{(t,x) : t > 0, x \in R^N\}$ the problem of Cauchy

$$Lu \equiv \frac{\partial u}{\partial t} - \nabla(k(t,x)u^{\sigma}\nabla u) - \varepsilon\gamma(t,x)u^{\beta} = 0 \tag{1}$$

$$u_{|t=0} = u_0(x) \geq 0, x \in R^N \tag{2}$$

Where $\varepsilon = \pm 1$, functions $\gamma(t,x) > 0$ $k(t,x) > 0$ in Q, the numerical parameters $\sigma > 0$, $\beta > 0$, $\nabla(.) = grad_x(.)$.
The problem (1), (2) describes a processes of a nonlinear diffusion reaction, heat conductivity, a filtration in liquid and a gas in a heterogenic media at a presence of an absorption ($\varepsilon = -1$) or a source $\varepsilon = +1$ that power is equal to $\gamma(t,x)u^{\beta}$. Investigation of qualitative properties of various type solutions of the problem (1), (2) when $k(t,x) = cons$, $\gamma(t,x) = 1$ had established by many authors and were received lot of nonlinear effects ([1-7] and references). The aim of this paper is to obtain conditions of global solvability, including the case of strong absorption $(0 < \beta < 1)$, the estimates of solutions for the having physical tense weak solutions and free boundaries, based on the method of nonlinear splitting [3-5], standard equations.

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Optimal Control of West Nile virus in mosquito, birds and humans

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West Nile virus (WNv) was detected for the first time in North America in 1999, and then spread prolifically within birds, with over 300 species can contribute to the spreading of the virus. Among these many species of birds, Corvids and non-corvids family of birds have different responses to the virus. We proposed a model for the transmission dynamics of WNv in the mosquito-bird cycle and human, putting in to consideration the two kind birds of bird populations: corvids and non-corvids. The model is extended to assess the impact of some anti-WNv control measures. For this paper, I will introduce the model and some results on the optimal control.

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Drift-oscillatory steering with the forward-reverse method for calculating the potential of mean force

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We present a method that enables the use of the nonequilibrium forward-reverse (FR) method of Kosztin et al. on a broader range of problems in soft matter physics. Our method, which we call the oscillating forward-reverse (OFR) method, adds an oscillatory steering potential to the constant velocity steering potential of the FR method. This enables the calculation of the potential of mean force (PMF) in a single unidirectional oscillatory drift, rather than multiple drifts in both directions as required by the FR method. By following small forward perturbations with small reverse perturbations, the OFR method is able to generate a piecewise reverse path that follows the piecewise forward path much more closely than any practical set of paths used in the FR method. We calculate the PMF for four different systems: a dragged Brownian oscillator, a pair of atoms in a Lennard-Jones liquid, a Na+ -Cl- ion pair in an aqueous solution, and a deca-alanine molecule being stretched in an implicit solvent. In all cases, the PMF results are in good agreement with those published previously using various other methods, and, to our knowledge, we give for the first time PMFs calculated by nonequilibrium methods for the Lennard-Jones and Na+ -Cl- systems.

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A hybrid modeling approach for option pricing

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The complexity of option pricing has led many researchers to develop sophisticated models for such purposes. The commonly used Black- Scholes model suffers from a number of limitations. One of these limitations is the assumption that the underlying probability distribution is lognormal and this is so controversial. We propose a couple of hybrid models to reduce these limitations and enhance the ability of option pricing. The key input to option pricing model is volatility. In this paper, we use three popular GARCH type model for estimating volatility. Then, we have developed two non-parametric models based on Neural Networks and Neuro-Fuzzy Networks to price call options for S&P 500 index. We have compared the results with those of Black- Scholes model and show that both Neural Network and Neuro-Fuzzy Network models outperform Black-Scholes model. Furthermore, comparing the Neural Network and Neuro-Fuzzy approaches, we observe that for at-the-money options, Neural Network model performs better and for both in-the-money and out-of-the money options, Neuro-Fuzzy model provides better results.

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Supervised Independent Component Analysis Based on Hilbert-Schmidt Independence Criterion

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Independent Component Analysis (ICA) is not only a method of exploring independent sources of a signal but also has become a popular method for feature extraction in different fields including finding of effective genes in a certain disease from DNA microarrays data set (see Ref. [1]). But when it is applied to identify the relevant genes, a set of linear basis vectors that are independent doesn't show satisfactory results. That's in part because ICA doesn't take advantage of class labels to find out the effective independent components of the data. Supervisd ICA is an idea to improve ICA in order to have independent components which are more related to the class labels.

Here we propose a supervised ICA algorithm which exploits Hilbert-Schmidt Independence Criterion (HSIC) to control the amount of changes of independent vectors that are explored at each step.Emperical estimation of Hilbert-Schmidt Independence Criterion is based on the following formula (see Ref. [2]):

$$HSIC := (n-1)^{-1} Tr(\mathbf{KHBH}) \tag{1}$$

where $\mathbf{H} = \mathbf{I} - n^{-1}\mathbf{1}\mathbf{1}^T$ and $\mathbf{K}$ and $\mathbf{B}$ are positive semidefinite kernel functions of random variables input x and lable y. The vector changes are chosen to be inversely proportional to their dependency to the class labels, as the goal is to find out independent vectors which are more relevant to the certain disease. The vectors that have more dependency to the class labels instead of changing a lot will be tuned slowly. But those which are less dependent will vary more in order to converge to the more appropriate independent vectors. This is estimated according to the following equation:

$$w^+ = w - \mu_i[\mathbf{E}\{xg(w^T x)\} - \beta w]/[\mathbf{E}\{g^{'}(w^T x) - \beta\}] \tag{2}$$

μ_i is equal to $\frac{1}{1+u_i}$ and u_i is a mapping vector which maximize Hilbert-Schmidt Independence criterion. In addition, in order to have a better starting point, the known vectors that have more dependency to the class data are passed as initial vectors. Our algorithm results in more reasonable number of genes that are known to be effective on the disease of our study. The percentage of meaningful gene achieved from the proposed algorithm is promising compared to ICA.

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Modelling The Relation Between Magnetic And Elastic Properties Of Magnetic Materials

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We study the interrelation between magnetization and density order parameters in ferromagnetic materials using a time dependent Ginzburg-Landau formalism i.e., we extend the free energy of the Phase Field Crystal model [1] to study how magnetic domains affect the microstructures in magnetic materials and vice versa. In our simulations, we used Finite Difference and Fast Fourier Transform methods to solve dynamical equations of motion. We also calculated the phase diagram of the model by minimizing the free energy in terms of the parameters of an approximate solution of the system and then applying the common tangent construction to find the equilibrium states. The results of the simulation are in agreement with the calculated phase diagram and let us analyze the effect of the magnetization-density coupling.

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Numerical Analysis of Time-Dynamic Multi-Phase Flow in Volcanic Conduits

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Time variability at the surface of an erupting volcano is often observed, yet there is little geological evidence of time variability within the magma chamber itself. In order to understand the nature of volcanic eruptions we develop fully time dynamic models of the multi-phase flow in the volcanic conduit. We consider the vertical flux of the magmatic-gas mixture in the conduit over time, with constant pressure within the magma chamber and at the peak of the lava dome. We approach the problem through a combination of linearized stability analysis and numerical computation. The stability of steady state solutions to the fully nonlinear multi-phase flow problem are examined and linearly unstable perturbations are then used as initial conditions for time-stepping the nonlinear model. We will also discuss changes of the stability properties as a function of changes to physical parameters. We aim to model the principle contributions to phase dynamics and stability, specifically dealing with time dynamic solutions.

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A Regression Algorithm for Compact Modeling of Multi-Dimensional Problems

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Model reduction is an approach for fast and cost-efficient modeling of large-scale systems governed by partial differential equations (PDEs). Model reduction is extended to multi-dimensions to reduce the linear system simultaneously with respect to frequency and any other parameter of the interest [1]. Multi-dimensional model reduction is also suggested for reduction of weakly nonlinear systems based on variational analysis and Volterra theory [2]. Multiple dimensions increase the size of reduced model and degrade the efficiency of reduction. In this paper a new methodology is proposed to efficiently build the reduced model based on regression analysis.

The Multi-dimensional computation of the reduced order model expands the transfer function into a multi-dimens- ional Taylor series expansion. Once all the orthonromalized moment coefficients with respect to different dimensions are evaluated, the multidimensional subspace $\mathbf{K}$ is constructed as $\mathbf{K} = [\mathbf{M}^1, \mathbf{M}^2, ...]$. The proposed algorithm measures the deviation between each vector in $\mathbf{M}^2$ with respect to orthonormalized vectors in base subspace $\mathbf{Q} = \mathbf{M}^1$. The minimum deviation for each vector in the second subspace with respect to the base subspace demonstrates the proximity of the resulting subspace to the base subspace. If the deviation is above the specified tolerances, then the moment will be added to subspace through an orthonormalization process as provided in Figure 1. Otherwise it will be removed from the subspace. For higher dimensions the subspace is integrated by repeating the algorithm in Figure 1 where the resulted $\mathbf{Q}$ form the pervious dimension is the base subspace.

As an example an electronic network with two coupled interconnects and one nonlinear pulse-shaping line is considered. The original model, sized 1386, is compared with reduced models using traditional and proposed approach, both sized 176 in Figure 2. The proposed method demonstrates a better accuracy than traditional approach.

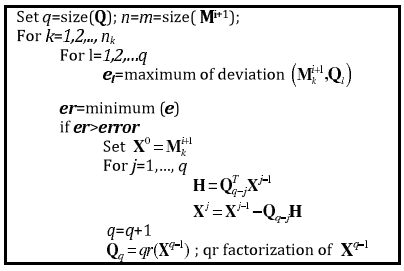

Figure 1: The regression algorithm.

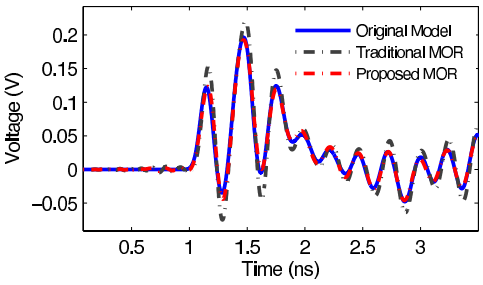

Figure 2: Weakly nonlinear results.

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Posterior Density Estimation for a Class of On-line Quality Control Models

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On-line quality control during production calls for a periodical monitoring of the produced items according to some prescribed strategy. Based on the quality requirements and limited by the cost a control region is pre-selected. If the examined item satisfies the control limits, the process is said to be in control and the production continues; otherwise, the process is declared out of control and the production is stopped for adjustments. At each stoppage a new production cycle is defined. It is reasonable to consider the existence of system internal non-observable variables so that the carried out monitoring is only partially reliable. It is assumed that the evolution of the internal state changes are governed by a finite-state Markov chain $\{\theta_n\}_{n\geq 0}$ and that jointly with the observable variables $\{X_n\}_{n\geq 1}$ we have a setting of a Hidden Markov Model. Two cases will be analysed. First, suppose that the transition matrix of $\{\theta_n\}$ as well as the conditional densities of X_n given θ_n are known, then the posterior density $p(\theta_n|x_{1:n})$ is estimated via particle filter type algorithms and convergence results are derived. Next, we assume that the transition probabilities of $\{\theta_n\}$ are unknown. Based on the observable sample $(X_1,\ldots,X_n) = x_{1:n}$ kernel density methods are used to approximate the stable regime density and to obtain estimates for false-alarm and non-detection malfunctioning probabilities.

Research partially supported by CNPq, CAPES, FAPDF and FINATEC.

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Plasmon Excitations in C_{60} by Fast Charged Particle Beams

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The study of collective electron excitations, or the so-called plasmons in nanometer sized structures is of great importance in many contemporary applications, including nano-optics, nano-electronics, and bio-chemical sensors [1]. In particular, carbon nano-structures, such as fullerene molecules, carbon nanotubes, and the recently isolated graphene have attracted considerable interest in the past several years. Plasmon excitations in those structures have been extensively studied by a variety of experimental techniques, including the Electron Energy Loss Spectroscopy (EELS) which uses electron beams with the incident energy on the order of 100 keV [2]. Carbon nano-structures in general, and the C_{60} molecule in particular are found to exhibit collective excitations of both their strongly bound σ electrons and the loosely bound π electrons.

In a recent theoretical study of carbon nanotubes, we have developed a two-dimensional, two-fluid hydrodynamic model which treats the σ and π electrons as two fluids constrained to move on a cylindrical surface [3]. In the present work, we adopt that model and apply it to a spherical cage representing the C_{60} molecule. We find that, like in the case of carbon nanotubes, spherical model also gives rise to splitting of the plasmon excitation frequencies into two groups, corresponding to collective modes of the π and σ electrons. Furthermore, we introduce phenomenological damping in the hydrodynamic model and evaluate the total cross section for inelastic electron scattering on C_{60} in gas phase in the semiclassical limit. The dependence of the cross section on electron energy loss is compared to the experimental EEL spectra of Ref.[2]

Moreover, following the procedure outlined in Ref.[3], we perform second quantization of plasmon oscillations within the two-fluid hydrodynamic model, enabling us to study multiple plasmon excitations in terms of both the electron energy and the point of incidence upon a C_{60} molecule. We find that the average numbers of dipole plasmons usually dominate at high incident energies and large distances but, at lower incident energies and for electron trajectories traversing the C_{60} molecule, the average numbers of multipolar plasmons become comparable to those of the dipole plasmons.

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A MULTI-DOMAIN HYBRID METHOD FOR HEAD-ON COLLISION OF BLACK-HOLES IN PARTICLE LIMIT

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A hybrid method is developed based on spectral and finite-difference methods for solving the inhomogeneous Zerilli equation in time-domain. The developed hybrid method decomposes the domain into the spectral and finite-difference domains. The singular source term is located in the spectral domain while the solution in the region without the singular term is approximated by the higher-order finite-difference method.

The spectral domain is also split into multi-domains and the finite-difference domain is placed as the boundary domain. Due to the global nature of the spectral domain, a multi-domain method only composed of the spectral domain does not yield the proper power-law decay unless the range of the computational domain is large. The finite-difference domain helps reduce boundary effects due to the truncation of the computational domain. The multi-domain approach with the finite-difference boundary domain method reduces the computational requirements significantly and also yields the proper power-law decay (see Fig. 1).

Stable and accurate interface conditions between the finite-difference and spectral domains and the spectral and spectral domains are derived. For the singular source term, we use both the Gaussian model with various values of full width at half maximum and a localized discrete δ-function. The discrete δ-function was generalized to adopt the Gauss-Lobatto collocation points of the spectral domain.

The gravitational waveforms from black hole ringdown are observed . Numerical results show that the developed hybrid method accurately yields the quasi-normal modes and the power-law decay profile. The numerical results also show that the power-decay profile is less sensitive to the shape of the regularized δ-function for the Gaussian model than expected. The Gaussian model also yields better results than the localized discrete δ-function.

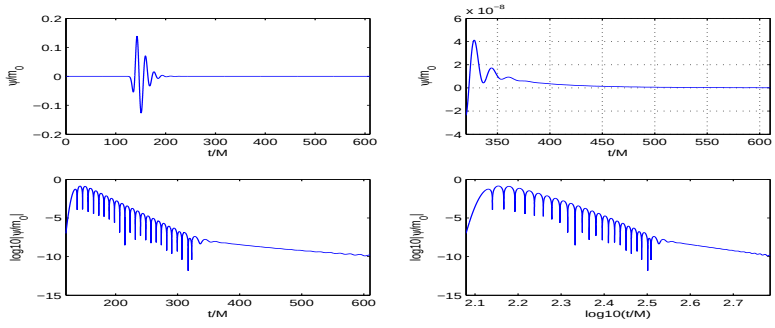

Figure 1: The Gravitational wave form and the power-law decay with the Gaussian model with $\sigma = 20$. $R_e = -300$, $R_\infty = 387.5$, $r_0 = 1.5(2M)$.

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Optimizing the performance of a hybrid method for numerically solving and visualizing vascular flows

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A large part of the human vasculature exhibits a streamline flow with no lateral mixing, but occasional turbulence can be witnessed near irregular geometric areas such as bifurcations, stenoses, and aneurysms. These can cause serious health problems which often require immediate surgical attention, and therefore it is important to be able to quickly obtain an accurate visualization of the blood flow near such areas. In order to make the diagnosis and treatment of blood vessels more successful by acquiring accurate models in optimal time, we employ a variety of enhancements and modern technological instruments.

We introduce an innovative method to hybridize the high-order spectral method - which needs a strict grid restriction for the complex geometry of a blood vessel - and the radial basis function (RBF) method - which is mesh-less and yields high-order accuracy for smooth problems. Hence, a complex geometry can be easily adopted while maintaining high-order accuracy. In order to make our method run as quickly as possible, we use the Python programming language coupled with Nvidias CUDA parallel computation application. Python is a powerful programming language with efficient high-level data structures and an intuitive approach to object-oriented programming. Its elegant syntax and dynamic typing make it an ideal language for scripting on most platforms. PyCUDA gives access to the CUDA programming interface from Python, which makes it much easier to write correct crash-free code, and unlocks the full potential of CUDA's driver API. In addition, PyCUDA's base layer is written in C++, which gives it the necessary speed to decrease the calculation times. Finally, we employ a Graphics Processing Unit which is a specialized circuit designed to rapidly manipulate and alter memory in order to accelerate the synthesis of images. Modern GPUs are very efficient at manipulating computer graphics, and their highly parallel structure makes them more adept than general-purpose CPUs for algorithms where processing of large blocks of data is done in parallel. Thus, this enables us to keep the processing times to a minimum.

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The International Conference on Applied Mathematics, Modeling and Computational Science
2011
ISBN: 2810000004711