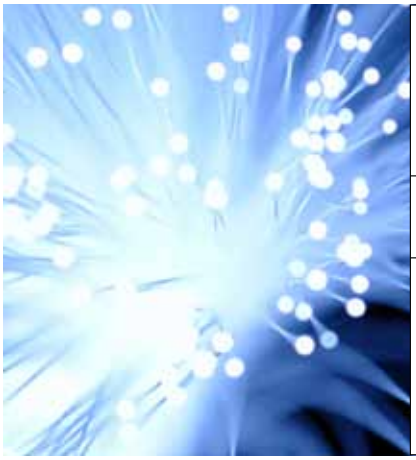
The INTERNATIONAL CONFERENCE on
APPLIED MATHEMATICS,
MODELING and COMPUTATIONAL SCIENCE



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BOOK OF ABSTRACTS

Technical Design by
Dalibor D Dvorski

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Waterloo, Ontario, Canada
August 26-30, 2013

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CS-CACO	Computational Algebra, Combinatorics and Optimization
CS-CPC	Computational Physics and Chemistry
CS-DSDE	Applications of Dynamical Systems and Differential Equations
CS-FINANCE	Financial Mathematics and Computation
CS-MECHE	Computational Mechanics and Engineering
CS-MODELING	Partial Differential and Integral Equations in Mathematical Modeling
CS-POST	Poster Session

Plenary Sessions

Models, Mathematics, and Markets - Is the Intersection an Empy Set?

Peter Carr (Morgan Stanley)

Did Albert Einstein ever write that compound interest is the most powerful force in the universe? I have my doubts, but the financial crisis of 2007-8 has left little doubt that mathematical models matter for markets. In this high-level talk, I will provide a historical overview of how mathematics has been used to model markets.

Dr. Peter Carr is a Managing Director at Morgan Stanley with over 15 years of experience in the financial industry. He is currently the Global Head of Market Modeling, overseeing several quantitative teams spread over three continents. He also presently serves as the the Executive Director of the Math Finance program at NYU's Courant Institute, the Treasurer of the Bachelier Finance Society, and a trustee for the Museum of Mathematics in New York. Prior to joining the financial industry, Dr. Carr was a finance professor for 8 years at Cornell University, after obtaining his PhD from UCLA in 1989. He has over 75 publications in academic and industry-oriented journals and serves as an associate editor for 8 journals related to mathematical finance. He was selected as Quant of the Year by Risk Magazine in 2003 and Financial Engineer of the Year by IAFE/Sungard in 2010. For the last two years, Dr. Carr has served on the CFTC's Technology Advisory Committee and was listed in Institutional Investor's Tech 50, an annual listing of the 50 most influential people in financial technology.

How Quantum Mechanics Can Help Solve the World's Energy Problems

Emily A. Carter (Princeton University)

If we are to survive as a species on this planet, we must make major science and engineering breakthroughs in the way we harvest, store, transmit, and use energy. An overview of my own research efforts in this direction will be given, including: optimizing materials to improve efficiency of turbine engines used for power generation and aircraft propulsion, characterizing combustion of biofuels and tritium incorporation in fusion reactor walls, optimizing mechanical properties of lightweight metal alloys for fuel-efficient vehicles, optimizing ion and electron transport in solid oxide fuel cell cathodes, and designing novel materials from abundant elements for photovoltaics and photoelectrodes to convert sunlight into electricity and fuels.

Fast and accurate quantum mechanics methods enabling the treatment of large biofuel molecules and mesoscale defects in metals that control mechanical properties will be briefly discussed. Then examples of key metrics we calculate to help design efficient new materials for photovoltaics, photocatalysts, and solid oxide fuel cells will be presented. These metrics point toward which dopants or alloys are likely to provide the most efficient energy conversion materials.

Professor Carter is the Founding Director of the Andlinger Center for Energy and the Environment at Princeton University and the Gerhard R. Andlinger Professor in Energy and the Environment, as well as Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics. Her current research is focused entirely on enabling discovery and design of molecules and materials for sustainable energy, including converting sunlight to electricity and fuels, providing clean electricity from solid oxide fuel cells, clean and efficient combustion of biofuels, optimizing lightweight metal alloys for fuel-efficient vehicles, and characterizing hydrogen isotope incorporation into plasma facing components of fusion reactors.

Professor Carter received her B.S. in Chemistry from UC Berkeley in 1982 (graduating Phi Beta Kappa) and her Ph.D. in Chemistry from Caltech in 1987. After a year as a postdoctoral researcher at the University of Colorado, Boulder, she spent the next 16 years on the faculty of UCLA as a Professor of Chemistry and later of Materials Science and Engineering. She moved to Princeton University in 2004. She holds courtesy appointments in Chemistry, Chemical Engineering, and three interdisciplinary institutes (PICSciE, PRISM, and PEI). The author of over 260 publications, she has delivered more than 400 invited lectures all over the world and serves on numerous international advisory boards spanning a wide range of disciplines. Her scholarly work has been recognized by a number of national and international awards and honors from a variety of entities, including the American Chemical Society (ACS), the American Vacuum Society, the American Physical Society, the American Association for the Advancement of Science, and the International Academy of Quantum Molecular Science. She received the 2007 ACS Award for Computers in Chemical and Pharmaceutical Research, was elected in 2008 to both the American Academy of Arts and Sciences and the National Academy of Sciences, in 2009 was elected to the International Academy of Quantum Molecular Science, in 2011 was awarded the August Wilhelm von Hoffmann Lecture of the German Chemical Society, and in 2012 received a Doctor Honoris Causa from the Ecole Polytechnique Federale de Lausanne.

Information Integration/Organization and Numerical Harmonic Analysis

Ronald R. Coifman (Yale University)

We provide an overview of recent developments in methodologies for empirical organization of data. We present a geometric/analytic mathematical framework for learning, which revolves around building a network or a graph whose nodes are observations. In our framework, connections between observations are constantly reconfigured in order to achieve learning for specific tasks. In particular we will provide a synthesis of a range of ideas from mathematics and machine learning, which address the transition from a local similarity model to a global configuration. This is analogous to Newtonian Calculus, which from of a local linear model of variability, calculates a global solution to a differential, or partial differential equation. We apply these fundamentals to jointly organize the rows and columns of a matrix, viewed either as the matrix of a linear operator, or as a Database. Here the rows are viewed as functions on the columns and the columns as functions of the rows, a dual geometry is built to optimize prediction and processing. We relate these methods to ideas from classical Harmonic Analysis and indicate tools to measure success of information extraction. In particular we introduce methodologies that resemble "signal processing" on data matrices, enabling functional regression, prediction, denoising, compression fast numerics, and so on. We illustrate these ideas to organize and map out in an automatic and purely data driven fashion on music databases of audio segments, text documents, psychological questionnaires, medical profiles, physical sensor data, financial data.

Ronald R. Coifman is Phillips professor of mathematics at Yale University. He received his Ph.D. from the University of Geneva in 1965. Prior to coming to Yale in 1980, he was a professor at Washington University in St Louis. Prof. Coifman's recent publications have been in the areas of nonlinear Harmonic Analysis , Fourier Analysis, wavelet theory, numerical analysis and scattering theory. Professor Coifman is currently leading a research program to develop new mathematical tools for efficient transcription and organization of data, with applications to feature extraction, learning classification and denoising. He was chairman of the Yale mathematics department 1986-89. He is a member of the National Academy of Sciences, American Academy of Arts and Sciences, and the Connecticut Academy of Sciences and Engineering. He received the DARPA Sustained Excellence Award in 1996, and the 1996 Connecticut Science Medal. The 1999 Pioneer award from the International Society for Industrial and applied Mathematics , the National Science Medal 1999, And the Wavelet Pioneer award 2009.

Data-driven Methods for Dynamical Systems: Quantifying Predictability and Extracting Spatiotemporal Patterns

Dimitrios Giannakis (New York University)
Andrew Majda (New York University)

Large-scale datasets generated by dynamical systems arise in many applications in science and engineering. Two research topics of current interest in this area involve using data collected through observational networks or output by numerical models to quantify the uncertainty in long-range forecasting, and improve understanding of the operating dynamics. In this talk we discuss applied mathematics techniques to address these topics blending ideas from machine learning, delay-coordinate embeddings of dynamical systems, and information theory. We illustrate these techniques with applications to climate atmosphere ocean science.

Dr. Dimitrios Giannakis is a faculty member at the Courant Institute of Mathematical Sciences, NYU. He is also affiliated with Courant's Center for Atmosphere Ocean Science (CAOS). He received BA and MSci degrees from the University of Cambridge, and a PhD degree from the University of Chicago. Prior to joining Courant and CAOS as faculty he was a postdoctoral researcher there. Giannakis' research work is at the interface between applied mathematics and climate atmosphere ocean science. His primary research interests are in geometrical data analysis algorithms and statistical modeling of complex systems. He has applied these tools in topics including idealized dynamical systems, ocean and sea ice variability on seasonal to interannual timescales, and organized atmospheric convection.

Andrew J. Majda is the Morse Professor of Arts and Sciences at the Courant Institute of New York University. Majda's primary research interests are modern applied mathematics in the broadest possible sense merging asymptotic methods, numerical methods, physical reasoning, and rigorous mathematical analysis.

Majda is a member of the National Academy of Sciences and has received numerous honors and awards including the National Academy of Science Prize in Applied Mathematics, the John von Neumann Prize of the Society of Industrial and Applied Mathematics, and the Gibbs Prize of the American Mathematical Society. He is also a member of the American Academy of Arts and Science. He has been awarded the Medal of the College de France, twice, and is a Fellow of the Japan Society for the Promotion of Science. He has received an honorary doctorate from his undergraduate alma mater, Purdue University.

In the past several years at the Courant Institute, Majda has created the Center for Atmosphere Ocean Science with a multi-disciplinary faculty to promote cross-disciplinary research with modern applied mathematics in climate modeling and prediction. Majda's current research interests include multi-scale multi-cloud modeling for the tropics, reduced stochastic and statistical modeling for climate, and novel mathematical strategies for prediction and data assimilation in complex multi-scale systems.

Patterns of Synchrony

Martin Golubitsky (Ohio State University)

This talk will survey recent results on rigid phase-shift synchrony in periodic solutions of coupled systems of differential equations. The mathematical questions were motivated by previous work on quadrupedal gaits and will be interpreted in terms of a generalized model for binocular rivalry.

Martin Golubitsky is Distinguished Professor of Natural and Mathematics Sciences at the Ohio State University, where he serves as Director of the Mathematical Biosciences Institute. He works in the fields of nonlinear dynamics and bifurcation theory studying the role of symmetry in the formation of patterns in physical systems and the role of network architecture in the dynamics of coupled systems. He has co-authored four graduate texts, one undergraduate text, and two nontechnical trade books.

Dr. Golubitsky is a Fellow of the American Academy of Arts and Sciences, AAAS, and SIAM. He is also the 2001 corecipient of the Ferran Sunyer i Balaguer Prize for The Symmetry Perspective and the recipient of the 2009 Moser Lecture Prize of the SIAM Dynamical Systems Activity Group. He has been elected to the Councils SIAM, AAAS, and AMS. Dr. Golubitsky was the founding Editor-in-Chief of the SIAM Journal on Applied Dynamical Systems and has served as President of SIAM.

Computer Involvement in the Classification of Small Index Subfactors

Vaughan Jones (Vanderbilt University)

A subfactor of index k is a generalisation of a permutation group on a set of size k. Except that the number k is no longer required to be an integer- it is a real number. While the listing of all transitive permutation groups on a set of size 5 would be covered in a first class in group theory, the subfactor result has only recently been completed thanks to Morrison, Peters, Snyder and many other authors. And their computers. The classification begins with the enumeration of all possible "Principal graphs", which in index less than or equal to 4 are the usual singly laced Coxeter graphs. Ten more subfactors exist with index between 4 and 5, some of which are only accessible via computer computations. I will present these results and the local blend of computer calculation and theory, and the extent to which the computer calculations may or may not be necessary.

Sir Vaughan F. R. Jones (KNZM FRS FRSNZ) is a New Zealand mathematician, known for his work on von Neumann algebras and Knot Theory. He was awarded a Fields Medal in 1990 at the ICM in Kyoto. Jones is currently a distinguished professor of mathematics at Vanderbilt University. He previously served as a professor at the University of California, Berkeley and a Distinguished Alumni Professor at the University of Auckland.

Nanocomputations by DNA Self-Assembly

Lila Kari (Western University)

Self-assembly, the process by which objects autonomously come together to form complex structures, is ubiquitous in the physical world: Atoms bind to each other to form molecules, molecules may form crystals or macromolecules, cells interact to form biological organisms. Recent experimental research in DNA self-assembly demonstrated its potential for the parallel creation of a large number of nanostructures, including some encoding computations. This suggests exciting applications of self-assembly to circuit fabrication, nanorobotics, DNA computation, smart-drug design, and amorphous computing.

A systematic study of self-assembly as a computational process has been initiated by Adleman and Winfree. The individual components are therein modelled as square tiles on the infinite two-dimensional plane. Each side of a tile is covered by a specific "glue", and two adjacent tiles will bind to each other if they have matching glues on their abutting edges. Tiles that stick to each other may form various two-dimensional structures such as squares, rectangles, counters, or may cover the entire plane. In this talk I will describe the potential of the self-assembly of "DNA tiles" for nanocomputations. In addition, I will explore generalizations of the original model that add the possibility of having negative, "repelling", glues, as well as compare the computational power of deterministic versus non-deterministic self-assembly.

Lila Kari is Professor in the Department of Computer Science at The University of Western Ontario. She received her M.Sc. in 1987 from the University of Bucharest, Romania, and her Ph.D. in 1991 for her thesis "On Insertions and Deletions in Formal Languages", for which she received the Nevanlinna Prize for the best mathematics thesis in Finland. Author of more than 170 peer reviewed articles, Professor Kari is regarded as one of the world's experts in the area of biomolecular computation, that is using biological, chemical and other natural systems to perform computations. She has served as Steering Committee Chair for the DNA Computing conference series, as Steering Committee member for the Unconventional Computation conference series, as well as on the Scientific Advisory Committee of the International Society for Nano-Scale Science and Engineering.

Lila Kari serves on the editorial boards of the journals Theoretical Computer Science, Natural Computing and Universal Computer Science, and as section editor for molecular computing for the Natural Computing Handbook (Springer). She has additionally served as a member of the Board of Directors of the FIELDS Institute for Research in Mathematical Sciences, the UK EPSRC peer review college, on the NSERC grant selection committee on computing and information systems and the NSERC Herzberg-Brockhouse-Polanyi Prize joint selection committee. At the University of Western Ontario she has received numerous awards, including the Florence Bucke Science Prize and the Faculty of Science Award for Excellence in Undergraduate Teaching. From 2002 to 2011 she was Canada Research Chair in Biocomputing, and her current research focusses on theoretical aspects of bioinformation and biocomputation, including models of cellular computation, nanocomputation by DNA self-assembly and Watson-Crick complementarity in formal languages.

Systemic Risk

George C. Papanicolaou (Stanford University)

The quantification and management of risk in financial markets is at the center of modern financial mathematics. But until recently, risk assessment models did not consider seriously the effects of interconnectedness of financial agents and the way risk diversification impacts the stability of markets. I will give an introduction to these problems and discuss the implications of some mathematical models for dealing with them.

George C. Papanicolaou is currently the Robert Grimmett Professor in Mathematics at Stanford University. Besides his former focus on the analysis of waves and diffusion in inhomogeneous or random media, his recent research interests also include financial mathematics, especially the use of asymptotics for stochastic equations in analyzing complex models of financial markets and in data analysis. In 1987, the University of Athens conferred an Honorary Doctor of Science on Papanicolaou. In 2000, he became a Fellow of the American Academy of Arts and Sciences and he was elected to the U.S. National Academy of Sciences. Papanicolaou was invited plenary speaker at multiple international congresses, among others at the SIAM 50th anniversary meeting in 2002 and at the International Congress of Industrial and Applied Mathematics in 2003. In 2006, he received the SIAM von Neumann Prize in recognition of his wide-ranging work on analytic and stochastic methods and their application to the modeling of phenomena in the physical, geophysical, and financial sciences. In 2010 he received the William Benter Prize in Applied Mathematics. In 2011 he was the Gibbs lecturer of the American Mathematical Society. The University of Paris Diderot conferred on him the degree Doctor Honoris Causa in 2011.

Optimization and Modeling in Energy Systems

Panos M. Pardalos (University of Florida)

For decades, power systems have been playing an important role in humanity. Industrialization has made energy consumption an inevitable part of daily life. Due to our dependence on fuel sources and our large demand for energy, power systems have become interdependent networks rather than remaining independent energy producers. This talk will focus on the problems arising in energy systems as well as recent advances in optimization and modeling to address these problems. Among the topics to be discussed are emission constrained hydrothermal scheduling, electricity and gas networks expansion, as well as reliability analysis of power grid.

Panos M. Pardalos serves as Distinguished Professor of Industrial and Systems Engineering at the University of Florida. He is also an affiliated faculty member of the Computer and Information Science Department, the Hellenic Studies Center, and the Biomedical Engineering Program. He is also the Director of the Center for Applied Optimization. Dr. Pardalos is a world leading expert in global and combinatorial optimization. His recent research interests include network design problems, optimization in telecommunications, e-commerce, data mining, biomedical applications, and massive computing.

Superconductivity and Automorphic Functions

Israel Michael Sigal (University of Toronto)

Macroscopic theory of superconductivity is based on the celebrated Ginzburg - Landau equations. First developed to explain and predict properties of superconductors, these equations had a profound influence on physics well beyond their original designation area. These are a pair of coupled nonlinear equations for a complex function (called order parameter or Higgs field) and a vector field (magnetic potential or gauge field). They are the simplest representatives of a large family of equations appearing in physics and mathematics. (The latest variant of these equations is the Seiberg - Witten equations.) Besides of importance in physics, they contain beautiful mathematics (some of the mathematics was discovered independently by A. Turing in his explanation of patterns of animal coats). In this talk I will review recent results involving key solutions of these equations - the magnetic vortices and vortex lattices, their existence, stability and dynamics, and how they relate to the modified theta functions appearing in number theory. Some automorphic functions play a key role in this theory.

Israel Michael Sigal is the Norman Stuart Robertson Chair in Applied Mathematics and University Professor at the University of Toronto. He works in several areas of mathematical physics. Among his results are the proof (jointly with Avy Soffer) of asymptotic completeness of the quantum many-body scattering for short-range potentials and the development of a mathematical framework (jointly with Volker Bach and Jurg Frohlich) of the theory of emission and absorption of quantum radiation by non-relativistic quantum systems such as atoms and molecules, as well as several important results on the nonlinear Schrodinger, Ginzburg-Landau, mean-curvature and wave equations. Professor Sigal was an invited speaker at several International Congresses of Mathematical Physics and at an International Congress of Mathematicians.

Phylogenetic Analysis of the Musical Rhythms of the World

Godfried T. Toussaint
(New York University, Massachusetts Institute of Technology, McGill University)

The application of computational-mathematical tools to the analysis of symbolically notated musical rhythms of the world informs musicological issues such as whether one group of rhythms is more complex than another, whether one family of rhythms possesses an underlying metrical hierarchy, or how an evolutionary phylogeny of musical rhythms may be constructed. Recent results on these problems will be illustrated with examples. To submit rhythms to a phylogenetic analysis, a measure of similarity between rhythms is usually employed.

Two fundamental approaches to measuring the similarity between rhythms are compared: a feature-based technique and a transformation method. In the former procedure, statistical and/or structural features are computed from a suitable representation of the rhythms, thus representing them as points in a feature space. Two rhythms are considered to be similar if the distance between their corresponding points in this feature space is small. In the latter strategy a rhythm is represented as a binary sequence of symbols denoting onsets (sounds) and rests (silences), and a distance measure called the edit-distance is used. The edit distance between two rhythms is the minimum number of mutations required to transform one rhythm to the other. Here the mutations consist of insertions, deletions, and substitutions of onsets and rests. A phylogenetic analysis using the BioNJ algorithm from the SplitsTree-4 software package, incorporating the edit distance, applied to several collections of the musical rhythms practiced in several cultures around the globe, yields new insights into the paradigmatic roles played by the most salient rhythms.

Godfried T. Toussaint is a Research Professor of Computer Science at New York University Abu Dhabi in Abu Dhabi, United Arab Emirates. He is also an affiliate researcher in the Computer Science and Artificial Intelligence Laboratory at the Massachusetts Institute of Technology in Cambridge, MA, USA. For many years he taught and did research in the School of Computer Science at McGill University in Montreal, in the areas of information theory, pattern recognition, textile-pattern analysis and design, computational geometry, machine learning, music information retrieval, and computational music theory. In 2005 he became a researcher in the Centre for Interdisciplinary Research in Music Media and Technology, in the Schulich School of Music at McGill University, in Montreal, Canada.

Dr. Toussaint is a founder and co-founder of several annual international conferences and workshops, including the ACM Symposium on Computational Geometry, and the Canadian Conference on Computational Geometry. He is an editor of several journals, including Computational Geometry: Theory and Applications, the International Journal of Computational Geometry and Applications, ISRN Geometry, and the Journal of Mathematics and the Arts. He is the recipient of several distinguished awards including a Killam Fellowship from the Canada Council for the Arts, and a Radcliffe Fellowship from Harvard University, where he spent one year at the Radcliffe Institute for Advanced Study, and one year in the Music Department. His research on the phylogenetic analysis of musical rhythms has been reported in several media, and was the focus of two Canadian television programs. He is the author of more than 390 publications.

Latest Book: The Geometry of Musical Rhythm, Chapman-Hall/CRC Press, January, 2013.

Semi-plenary Sessions

The Spatio-temporal Spread of Drug-resistant Tuberculosis

Julien Arino (University of Manitoba)

Tuberculosis is, after HIV/AIDS, the second largest cause of infectious disease induced death. It is estimated that in 2011, it killed 1.4 million people worldwide. Tuberculosis is also a disease of poverty, as contributing factors to its spread include poor and overcrowded living conditions, poor health conditions, etc. As a consequence, over 95\% of new infections and deaths by tuberculosis occur in developping countries.

We formulate a model for tuberculosis in a single population that includes three strains: a drug-sensitive strain, MDR-TB and XDR-TB. We study the model mathematically and show, in particular, that the bifurcation structure of the whole model is governed by the behaviour of the XDR-TB strain. We then extend the model to a metapopulation setting, in which each country is a vertex in a multi-digraph, endowed with a system for the single population case. Weighted arcs between the vertices represent the rate of travel of individuals between the countries. We study the resulting large-scale system. Finally, we proceed to numerical experiments with realistic travel and population data.

This is a joint work with K. Khan (University of Manitoba) and I. Soliman (St Michael's Hospital, Toronto).

Julien Arino received his PhD in 2001 from Universite Joseph Fourier in Grenoble, France in affiliation with INRIA Sophia Antipolis and the Villefranche-sur-mer Oceanological Observatory. He held postdoctoral fellowships at the University of Victoria (Jan 2001-Dec 2002) and McMaster University (Jan 2003-Jun 2005).

Since 2005, he has been a faculty member at the University of Manitoba. He is currently a member of the Bio.Diaspora Project, which is based at St Michael's Hospital (Toronto), and the Centre for Disease Modelling, which is hosted at York University.

Fair Division

Steven Brams (New York University)

Over the past 20 years, there has been burgeoning interest in the subject of fair division - how one divides a single divisible good (e.g., a cake), or multiple indivisible goods (e.g., the marital property in a divorce), to satisfy such properties as efficiency, envy-freeness, and equitability. Some of the major possibility and impossibility results -- relating to both the existence of such a division and algorithms for producing it - will be reviewed. How these results apply to dividing land, allocating items in a family estate to heirs, determining which rooms housemates get and how much of the rent each pays for its room, and matching applicants to colleges will be among the applications discussed.

Steven J. Brams is Professor of Politics at New York University and the author, co-author, or co-editor of 18 books and more than 250 articles. His books include Theory of Moves (Cambridge, 1994) and, co-authored with Alan D. Taylor, Fair Division: From Cake-Cutting to Dispute Resolution (Cambridge, 1996) and The Win-Win Solution: Guaranteeing Fair Shares to Everybody (Norton, 1999). His newest books are Mathematics and Democracy: Designing Better Voting and Fair-Division Procedures (Princeton, 2008) and Game Theory and the Humanities: Bridging Two Worlds (MIT, 2011). He holds two patents for fair-division algorithms and is chairman of the advisory board of Fair Outcomes, Inc.

Brams has applied game theory and social-choice theory to voting and elections, bargaining and fairness, international relations, and the Bible, theology, and literature. He is a former president of the Peace Science Society (1990-91) and of the Public Choice Society (2004-2006). He is a Fellow of the American Association for the Advancement of Science (1986), a Guggenheim Fellow (1986-87), and was a Visiting Scholar at the Russell Sage Foundation (1998-99).

On an Inverse and Ill-Posed Problem of Autoconvolution Type in Ultrashort Laser Pulse Characterization

Bernd Hofmann (Technical University of Chemnitz)

In the early 1990s motivated by applications from spectroscopy and stochastics contributions to the mathematical analysis of deautoconvolution problems as a class of inverse problems in spaces of continuous or quadratically integrable real functions were made. Such deautoconvolution problems were mostly aimed at finding non-negative functions with compact support from observations of its autoconvolution. Since the autoconvolution operator is nonlinear and smoothing, the deautoconvolution problem is ill-posed in the sense that the solutions need not be uniquely determined and mainly small perturbations in the data may lead to arbitrarily large errors in the solution. To overcome the negative consequences of ill-posedness some kind of regularization is required. Recently, the research group `Solid State Light Sources' of the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, hit on the autoconvolution problem in the context of a new approach in ultrashort laser pulse characterization called Self-Diffraction SPIDER. For phase reconstruction as an auxiliary problem the solution of an autoconvolution equation is needed, but now for complex functions to be determined from complex observations. Moreover, a device-related kernel function must be added. The ill-posedness phenomenon arises in the complex case, too, but a thorough analysis of the complex case in deautoconvolution was missing in the literature. The talk presents analytical and numerical results on the character of ill-posedness of the equation occurring as a part of the SD SPIDER approach. Moreover, an iterative regularization approach is suggested for the problem when only noisy data of are given.

Dr. Bernd Hofmann is professor for Analysis and Inverse Problems at the Chemnitz University of Technology, Germany, in the Department of Mathematics since 1993, where he served as Dean of the Faculty from 2006 to 2009. He established an interdisciplinary research group on inverse problems with applications in natural sciences, engineering and finance, organizing the annual `Chemnitz Symposium on Inverse Problems', sometimes on tour (in Linz 2009, Canberra 2012, and Shanghai 2013).

Dr. Hofmann's research focus is on regularization theory and practice as well as on studies concerning the nature of ill-posedness and appropriate tools for the treatment of ill-posedness phenomena. He works as a member of the Editorial Board of the journals `Inverse Problems' and `Journal of Inverse and Ill-Posed Problems'.

Ecological and Epidemiological Drivers of Viral Evolution

Eili Klein (John Hopkins University)

While it has long-been recognized that disease transmission is impacted by human behavior, the consequences of human behavior on the ecology of directly transmitted pathogens has been understudied. Using a biophysical model of virus stability, we examine how much of virus evolution is driven by epidemiological factors, such as contact rates and protective behavior, and how much is driven by biological characteristics of the virus, such as its growth rate. We use agent-based models, which scale from local to planetary to elucidate the driving factors for both endemic and epidemic directly transmitted viruses.

Dr. Eili Klein is an assistant professor at John Hopkins University in the Centre for Advanced modeling in the Social, Behavioural and Health Sciences; Dr. Klein also holds a fellow position at the Center for Disease Dynamics, Economics and Policy, in Washington, D.C. He received his PhD in ecology and evolutionary biology from Princeton University and has held research associate positions at the Center for Disease Dynamics, Economics and Policy and Resources for the Future.

Dr. Klein's interdisciplinary research involves ecology, epidemiology, economics, and human behaviour. His scientific interests include: factors that drive antimicrobial drug resistance; economic epidemiology; how human behaviour influences ecology/epidemiological dynamics; and how human behaviour influences evolution of an infectious disease.

Variational Principles in Wave-Functional and Density-Functional Formulations of Quantum Mechanics

Mel Levy (Duke University)

Variational theorems are important for obtaining approximate solutions to the Schroedinger equation. With this in mind, fundamental variational principles will first be discussed within the wave-functional formulation of quantum mechanics. Then the corresponding variational principles for ground states in density and density-matrix functional theories will be reviewed briefly for the non-degenerate and degenerate situations. Based on these variational principles, properties of the exact functionals will be presented that are difficult to satisfy with approximate functionals. Special emphasis will be given to degeneracies, coordinate scaling, and potentials (functional derivatives). Then, a new time-independent density-functional theory for excited states will be presented for Coulomb systems. The lecture will conclude with a description of certain relevant unsolved mathematical problems, such as one involving an ionization energy convexity property.

Professor Emeritus, Tulane University and North Carolina A\&T State University. Visiting Professor, Duke University (2007-). Professor, North Carolina Agricultural and Technical State University, 2002-2007. Professor, Tulane University, 1976-2002 (presently, Professor Emeritus). Visiting Professor or Visiting Scientist: Oak Ridge National Laboratory; Quantum Theory Project, University of Florida; Instituto Venezolano de Investigaciones Cientificas (I.V.I.C.), Caracas, Venezuela; Institute for Theoretical Physics, University of California at Santa Barbara; Institute of Theoretical Physics, Kossuth Lajos University, Debrecen, Hungary; Department of Physics and Theory Center Cornell University; Lecturer, Department of Chemistry, the University of North Carolina at Chapel Hill, 7/74-7/76.

International Academy of Quantum Molecular Science; International Academy of Mathematical Chemistry; Fellow of The American Physical Society; Editorial Board, Advances in Quantum Chemistry; Advisory Editorial Board, Theoretical Chemistry Accounts; Advisory Editorial Board, Progress in Theoretical Chemistry; Guest Editor: The International Journal of Quantum Chemistry; Tulane Liberal Arts and Sciences, Faculty Research Award, 1998.

Role of Dipolar Interactions in Protein Folding

Silvina Matysiak (University of Maryland)

The role of dipole interactions in protein folding A generic coarse-grained (CG) protein model will be presented to characterize the driving forces behind protein folding. The change in orientation of the atoms in the coarse-grained unit is captured by the addition of Drude oscillators inside each polar coarse-grained bead. The addition of dummy sites inside the polar beads introduces structural polarization into the coarse-grained model.

Realistic alpha/beta content is achieved de novo without any biases in the force-field toward a particular secondary structure. The dipoles created by the Drude oscillators interact with each other and drive the protein models to fold into unique structures depending on the amino acid patterning and presence of capping residues. In this talk, we will show the role of dipole-dipole and dipole-charge interactions in shaping the secondary and tertiary structure of proteins. In particular, we will focus on the folding of beta-hairpins and single helices and in helix bundles and multiple beta-sheet strands. In the folded ensemble, dipoles along a helix are found aligned parallel and stabilized by the presence of charged capping residues. On the other hand, beta-sheets exhibit antiparallel neighboring dipoles.

Dr. Silvina Matysiak is an assistant professor in the Fischell Department of Bioengineering at the University of Maryland College Park. She received her B.S. in Chemical Engineering from the Instituto Tecnológico de Buenos Aires in 2001 and her PhD in Chemistry from Rice University in 2007. Before joining Maryland, she was a postdoctoral fellow at the University of Texas at Austin.

Matysiak's primary area of interest is the characterization of protein dynamics and function at the molecular level. Her work includes using computer simulations to study the mechanism of protein folding and misfolding associated with neurodegenerative diseases, development of multiscale simulation approaches to bridge different time- and length-scales and how solvent organization affects cooperative transitions in biomolecular systems.

Boundary Conditions for Constrained Hyperbolic Systems: Mathematical and Numerical Analysis

Nicolae Tarfulea (Purdue University)

Many applications in sciences and technology lead to first order symmetric hyperbolic (FOSH) systems of differential equations supplemented by constraint equations. The Cauchy problem for many such FOSH systems is constraint-preserving, i.e., the solution satis?es certain spatial differential constraints whenever the initial data does (e.g., Maxwell's equations or Einstein's field equations in various FOSH formulations). Frequently, artificial space cut offs are performed for such evolution systems, usually out of the necessity for finite computational domains. However, it may easily happen that boundary conditions at the artficial boundary for such a system lead to an initial boundary value problem which, while well-posed, does not preserve the constraints. Therefore, boundary conditions have to be posed in such a way that the numerical solution of the cut off system approximates as best as possible the solution of the original problem on infinite space, and this includes the preservation of constraints. It has become increasingly clear that in order for constraints to be preserved during evolution, the boundary conditions have to be chosen in an appropriate way. Here we consider the problem of finding constraint-preserving boundary conditions for constrained FOSH systems in the well-posed class of maximal nonnegative boundary conditions. Based on a characterization of maximal nonnegative boundary conditions, we discuss a systematic technique for finding such boundary conditions that preserve the constraints, pending that the constraints satisfy a FOSH system themselves. We exemplify this technique by presenting a few relevant applications (e.g., for FOSH formulations of Einstein's equations and for systems of wave equations in FOSH formulation subject to divergence constraints).

Dr. Nicolae Tarfulea is Associate Professor in the Department of Mathematics, Computer Science \& Statistics, Purdue University Calumet. He received his PhD from the University of Minnesota and his M.S. in Mathematics from the Penn State University in 2004 and 2001, respectively. His main research Interests are in Partial Differential Equations; Numerical Analysis; General Relativity. More precisely: boundary conditions for hyperbolic formulations of Einstein's equations, nonlinear elliptic equations, reaction diffusion systems, compressed sensing, and finite element methods. He has published 23 papers on these subjects in some of the most prestigious journals of mathematics, and gave over 20 invited talks in the last five years, and been a part of six research grants.

Martini Coarse-grained and Atomistic Simulations of Lipids

Peter Tieleman (University of Calgary)

Computer simulations have been widely used to study properties of lipid aggregates. Over the past twenty years simulations have progressed from small models of lipid bilayers composed of one type of lipid at length scales of 5-8 nanometer and time scales of nanoseconds to very complex models at length scales of tens of nanometers and time scales of microseconds. The development of realistic coarse-grained models such as the MARTINI model has brought simulations of lipids to mesoscope scales where particle-based simulation and continuum models overlap and simulations can be compared to measurable mechanical parameters of lipid aggregates. MARTINI is parameterized primarily based on experimental data, but for many systems of biological importance there is limited experimental data that can be used in parameterization and validation. I will discuss recent progress in linking atomistic simulations, experimental results, and parameters from continuum models to MARTINI simulations, illustrated with examples on lipid mixtures, membrane tethers, and lipid-protein systems.

Peter Tieleman studied physical chemistry at the University of Groningen in the Netherlands, where he obtained his PhD under the supervision of Herman Berendsen, one of the pioneers of biomolecular simulation. After a year as a European Molecular Biology Organization fellow at the University of Oxford in Mark Sansom's research group, Tieleman joined the University of Calgary. Since 2005, he has been a Professor in the Department of Biological Sciences. His research interests are in biomolecular simulation and computational biology, with an emphasis on biochemical and biophysical problems involving cell membranes. Among his distinctions are an Alfred P. Sloan Foundation Fellowship, the Royal Society of Canada's Rutherford Memorial Medal in Chemistry, and a Natural Sciences and Engineering Research Council of Canada (NSERC) Steacie Memorial Fellowship.

Special Invited Speaker

Fifteen Years of Funded Programs to Advance Women in Science and Engineering: Progress and Persistent Challenges

Catherine Mavriplis (University of Ottawa)

I will discuss my work in advancing women in science and engineering through US National Science Foundation funding since 1997 and, more recently, since 2011, Canada's Natural Sciences and Engineering Research Council Chair for Women in Science and Engineering program. The FORWARD to Professorship program, in particular, has been a successful vehicle to empowering doctoral women who consider academic careers. Results of a survey of all 1300 FORWARD participants since 2003 will be presented, giving a picture of how this group of talented and motivated women are advancing and how the climate is changing. My work in Canada has also included women in industry, in particular with the Chair sponsor, Pratt & Whitney Canada, an aircraft engine manufacturer based in Montreal. I will discuss activities designed for mid-career professional women in industry as well as some initiatives for boosting numbers of women in computing.

Catherine Mavriplis, PhD, PE is an Associate Professor of Mechanical Engineering at the University of Ottawa and the NSERC Chair for Women in Science and Engineering (Ontario region). Dr. Mavriplis has been a professor of Mechanical and Aerospace Engineering since 1991, primarily at the George Washington University in the United States. She has also worked at the US National Science Foundation (NSF) in Mathematics and the University of Oklahoma in Meteorology. Her specialization is in Computational Fluid Dynamics and through application of her numerical modeling skills she has been involved in a number of interdisciplinary projects.

She maintains a strong collaboration with several U.S. researchers and the Royal Institute of Technology in Sweden. She currently serves on the Board of Directors of the Computational Fluid Dynamics Society of Canada. Dr. Mavriplis has worked under NSF funding to advance women since 1996, notably through the FORWARD to Professorship workshops under the NSF ADVANCE program, reaching up to 1,300 science and engineering doctoral women by 2013.

Special Symposia & Minisymposia

Applied Analysis and Inverse Problems (SS-AAIP)

Organizers:
Herb Kunze (University of Guelph)
Kimberly Levers (University of Guelph)

A typical inverse problem seeks to find a mathematical model that admits given observational data as an approximate solution. This sort of quesion is of great interest in many application areas, including mathematical ecology, environmental systems, physical systems, and image science, often appearing in the form of a parameter esimation problem. This session focuses on the applied analysis related to such inverse problems. The talks in the session will also include aspects of numerical analysis, mathematical modeling, and computational methods.

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A Novel Image Registration-Reconstruction Framework for Real-Time Monitoring of Paraspinal Tumors in Radiation Therapy

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The treatment of paraspinal tumors by stereotactic body radiation therapy (SBRT) represents a particular challenge due to the close proximity between the vertebral column and the spinal cord. Image-guided radiation therapy (IGRT) takes advantage of real-time imaging to help the delivery of more accurate radiation treatment.

From tomographic projections measured on a fluoroscopic flat panel at different gantry angles, we desire to design a real-time monitoring system of the patient position. This kind of problem is generally solved with a 2D-3D image registration algorithm between projections and the treatment planning CT volume or by first reconstructing a 3D volume and then performing 3D image registration. Unfortunately, direct 2D-3D image registration is not accurate enough for the detection of out-of-plane movements and the acquisition of all the projections for a full 3D reconstruction is too time consuming.

In this talk, we present a novel combined image registration-reconstruction framework for the monitoring of the patient motion during radiation therapy. The patient motion is estimated by solving the following equation

$$\arg\min_{\mathbf{x},\lambda} \{S(T_\lambda(\mathbf{z}),\mathbf{x}) + R(A\mathbf{x},\mathbf{p})\}, \tag{1}$$

where $\mathbf{p} \in \mathbf{R}^{KM}$ are K acquired projections of dimension M, stacked in a vector, $\mathbf{x} \in \mathbf{R}^N$ is the reconstructed volume, $\mathbf{z} \in \mathbf{R}^N$ is the planning CT volume on which the radiation treatment is based, T_λ is a transformation operator parameterized by λ, $A \in \mathscr{M}_{MK\times N}$ is a (linear and sparse) projection operator, S is an image similarity measure and R is a residual term associated with the noise model.

When $\mathbf{x} = T_\lambda(\mathbf{z})$, the problem simplifies to $2D-3D$ image registration (for $K=1$) or joint $2D-3D$ image registration (for $K>1$). On the other hand, when T_λ is fixed the problem simplifies to an algebraic reconstruction with the image similarity $S(T_\lambda(\mathbf{z}),\mathbf{x})$ as the regularizer. In particular, if we consider the simple case with the Euclidean distance as the similarity measure S and additive white Gaussian noise of variance σ^2 as the noise model R, then the problem simplifies to the well-known Tikhonov regularization and the solution is

$$\mathbf{x}^* = (A^TA + I/\sigma^2)^{-1}(A^T\mathbf{p}/\sigma^2 + T_\lambda(\mathbf{z})). \tag{2}$$

We thus propose to solve the joint reconstruction-registration problem by first reconstructing $\mathbf{x}$ algebraically for a given choice of parameter λ and then optimizing over the parameters of the transform T_λ. We consider in particular a three-dimensional rigid registration operator T_λ parameterized by $\lambda = (t_x, t_y, t_z, r_x, r_y, r_z)$, since this is the only type of transformation that can be corrected with a robotic treatment couch.

We will construct the forward operator A by considering the geometry of the problem and by performing trilinear basis interpolation. We will also present and solve for different noise models such as Gaussian or Poisson noise and different image similarity models such as the Euclidean distance and a variance-normalized Euclidean distance also known as the Structural Similarity index.

Numerical results on synthetic data, on phantoms as well as on clinical medical images will be presented.

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On the Application of Adjoint Methods in Subsurface Flow Simulations

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Application of the adjoint method to subsurface characterization will be presented. The model problem that the method will be applied to is the infiltration of water in soil. It is assumed that there is some measurement data available in the domain of interest and we would like to infer the subsurface permeability conditioned to the measurement data. A possible permeability field is proposed as a starting point for an iterative procedure. A simulation is completed using the proposed field and the results are then compared with the measurement data with the goal of finding a permeability field which will minimize the difference between the simulation and measurement data. At each iteration, the difference between the simulated results and measurement data is used to compute an update to the proposed field. The iteration is continued until some convergence criteria has been reached. Numerical examples demonstrating the method will be presented.

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A Scientific Way to Simulate Pattern Formation in Reaction-Diffusion Equations

E.A. Cleary[1]

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A large body of current literature in developmental biology, chemistry and applied mathematics focuses on the investigation of diffusion-induced instability ('Turing mechanism' [1]) in coupled reaction-diffusion equations. The general form of a coupled reaction diffusion equation is as follows,

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + f(u,v),\ \frac{\partial v}{\partial t} = D_v \nabla^2 v + g(u,v),$$

where D_u and D_v are positive diffusion coefficients and $u = u(x,y,t)$ and $v = v(x,y,t)$. Diffusion-induced instability occurs when a spatially homogeneous solution satisfying the coupled ordinary differential equation (ODE),

$$\frac{du}{dt} = f(u,v),\ \frac{dv}{dt} = g(u,v),$$

becomes linearly unstable with the presence of diffusion. For a uniquely defined subset of phase space the interaction of reaction and diffusion leads to stationary pattern formation phenomena, complex and organic in appearance. The solutions of these systems must often be analyzed numerically. The standard approach in the literature for approximating Turing systems uses finite difference, or finite element methods. Initial data equal to the equilibrium solutions of the corresponding ODE system are randomly perturbed at every point on the computational grid, which allows the Turing mechanism to kick-in and produce a pattern. The problem with such an approach is that resulting solutions are sensitive to initial conditions [2]. Furthermore, researchers typically use unspecified pseudo random number generators (RNG) with unspecified 'seeds' and do not always give full details of the computational grids used. As a result, reproducibility of solutions becomes an issue. Furthermore, the standard method of simulation does not facilitate the demonstration of convergence to a solution of the problem via the method of mesh refinement, as each grid effectively represents a different set of initial conditions. We explore a new methodology, which is independent of the choice of programming language, circumventing the aforementioned issues. While the new method allows more control over solutions, the user is required to make more choices, which may or may not have a determining effect on the nature of resulting patterns. In an attempt to quantify the extent of the possible effects, we study heterogeneous steady states for two well know reaction-diffusion models, the Gierer-Meinhardt model [4] and the Schnakenberg model [3].

This is joint work with M. Garvie and H. Kunze, Mathematics and Statistics, University of Guelph.

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Iterative Techniques for Nonlinear Periodic Boundary Value Problems via Initial Value Problems

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Since periodic boundary value problems (PBVPs, for short) are problems at resonance, the conditions required to construct iterative techniques for such problems are more stringent than those for the initial value problems (IVPs). In this talk, we design two types of iterative technique for the following nonlinear PBVP in the unified setting

$$u'(t) = f(t,u(t)) + g(t,u(t)) \text{ with } u(0) = u(T), \text{ for } t \in [0,T]. \tag{1}$$

The first method employed, the Monotone Iterative Technique (see Refs. [1, 3, 4]), has a linear mode of convergence. The rate of convergence of the second, the Generalized Quasilinear Technique (Refs. [2, 5]), is quadratic and hence more rapid. We employ natural lower-upper solutions and coupled lower-upper solutions in our investigations.

The interesting feature of our methods is that the iterates, which are solutions of linear IVPs, converge monotonically and uniformly to solutions of the given nonlinear PBVP. This fact allows us to impose minimal conditions on the forcing functions f and g in the given Eq. (1). The proofs of our results are also simpler than those of the conventional methods. We provide numerical and graphical illustrations of our results.

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Gravitational Wave Parameter Estimation with Compressed Likelihood Evaluations

P. Canizares[1], S. E. Field[2], J. R. Gair[3], M. Tiglio[4]

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One of the main bottlenecks in gravitational wave (GW) astronomy is the high cost of performing Bayesian parameter estimation. We propose a novel technique based on Reduced Order Quadratures (ROQs) [1], an application and data-specific quadrature rule, to perform fast and accurate likelihood evaluations. Generation of an ROQ rule is carried out offline (before the data is known). First, a projection-based greedy algorithm identifies a basis whose span accurately approximates the parameterized functions defining a GW model. An empirical interpolation procedure is then applied to select ROQ nodes. The resulting quadrature rule's computational cost depends linearly on the number of basis functions and, more precisely, the ROQ error is bounded by the model's Kolmogorov n-width times a computable constant.

For noisy data taken at equally spaced intervals numerical approximation of likelihood evaluations are computed by a low-order Riemann sum. ROQs are shown to converge exponentially fast thereby significantly accelerating these evaluations. Likelihood evaluations are the dominant cost in Markov chain Monte Carlo algorithms, which are widely employed in parameter estimation studies, and so ROQs offer a new way to accelerate GW parameter estimation.

We illustrate our approach using a four dimensional GW burst model embedded in large, Gaussian noise [2]. We build an ROQ for this model, and perform four dimensional MCMC searches with both the standard and ROQs quadrature rules, showing that, for this model, the ROQ approach is around 25 times faster than the standard approach with essentially no loss of accuracy. The speed-up from using ROQs is expected to increase for more complex signals and therefore has significant potential to accelerate parameter estimation of GW sources such as compact binary coalescences.

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On an Inverse and Ill-Posed Problem of Autoconvolution Type in Ultrashort Laser Pulse Characterization

B. Hofmann[1], D. Gerth[2], S. Birkholz[3], S. Koke[3], G. Steinmeyer[3]

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In the early 1990s motivated by applications from spectroscopy and stochastics contributions to the mathematical analysis of deautoconvolution problems as a class of inverse problems in spaces of continuous or quadratically integrable real functions were made (see, e.g., [1]). Such deautoconvolution problems were mostly aimed at finding non-negative functions x with compact support $\mathrm{supp}(x) \subset \mathbf{R}$ from its autoconvolution $y = x * x$. Since the autoconvolution operator $x \mapsto x * x$ is nonlinear and 'smoothing', the deautoconvolution problem is ill-posed in the sense that for given y the solutions x need not be uniquely determined and mainly small perturbations in the right-hand side y caused by noisy data may lead to arbitrarily large errors in the solution. To overcome the negative consequences of ill-posedness some kind of regularization is required.

Recently, the research group 'Solid State Light Sources' of the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, hit on the autoconvolution problem in the context of a new approach in ultrashort laser pulse characterization called Self-Diffraction SPIDER (cf. [2]). For phase reconstruction as an auxiliary problem the solution of an autoconvolution equation is needed, but for complex functions $x : [0,1] \subset \mathbf{R} \to \mathbf{C}$ to be determined from complex observations $y : [0,2] \subset \mathbf{R} \to \mathbf{C}$. The ill-posedness phenomenon arises in the complex case, too, but a thorough analysis of the complex case in deautoconvolution was missing in the literature. On the other hand, a device-related kernel function $k : [0,2] \times [0,1] \to \mathbf{C}$ involved in the mapping $x \mapsto y$ constitutes a challenging additional difficulty in connection with this inverse problem behind SD SPIDER. We present results on the character of ill-posedness of the equation

$$\int_0^s k(s,t)\, x(s-t)\, x(t)\, dt \;=\; y(s), \qquad 0 \le s \le 2, \tag{1}$$

occurring as a part of the SD SPIDER approach. Moreover, we suggest an iterative regularization approach for the problem when only noisy data of y are given. Numerical experiments with synthetic data based on realistic solution and kernel structures outline the opportunities and limitations of the method (see also [3] and [4]).

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On Set-valued Nonlinear Fredholm Integral Equations

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The nonlinear Fredholm integral equation

$$x(t) = f_0(t) + \int_0^1 f(t,s,x(s))ds \tag{1}$$

is studied in many different applied mathematical areas. For instance, in image applications x represents an input signal (or image), the function f involves a kernel that describes how the signal has been blurred, and the term f_0 represents the contribution of additive noise. Another research area in which such an equation arises is the analysis of two-point boundary value problems with certain non-linear boundary conditions.

In this work, we study a related set-valued nonlinear Fredholm integral inclusion

$$x(t) \in f_0(t) + \int_0^1 F(t,s,x(s))ds \tag{2}$$

where $f_0 : [0,1] \rightrightarrows \mathbb{R}^N$ and $F : [0,1] \times [0,1] \times \mathbb{R}^N \rightrightarrows \mathbb{R}^N$ are set-valued mappings, and $x : [0,1] \to \mathbb{R}^N$ is the unknown solution that has to be determined. Such integral inclusions arise when modeling systems for which we have no complete description.

We prove the existence of a solution and provide a method for determining an approximate solution based on the Steiner selection and the use of Schauder bases. We also discuss an inverse problem in the case when (2) is interval-valued.

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Changes in Habitat of Fish Populations: An Inverse Problem

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Mathematical modelling applies to a wide variety of application areas, and is an active area of research in many disciplines. It is often the case that accurate depiction of these phenomena require increasingly complex models. Unfortunately, this increased complexity in a model causes great difficulty when finding solutions. What is more, developing a model with known parameters that produces results consistent with observed behaviours may prove to be a difficult or even impossible task. These difficulties have brought about an interest in inverse problems.

A goal of many inverse problems is to find unknown parameter values, $\lambda \in \Lambda$, so that the given observed data u_{true} agrees well with the solution data produced using these parameters u_λ. Unfortunately finding u_λ in terms of the parameters of the problem may be a complex task. Further, the objective function may be a complicated function of the parameters $\lambda \in \Lambda$ and may require complex minimization techniques. In recent literature, the collage coding approach to solving inverse problems has emerged. This approach avoids the aforementioned difficulties by bounding the approximation error above by a more readily minimizable distance, thus making the approximation error small. In this talk, we utilize a collage-based approach to solving an inverse problem for a model for the migration of three fish species through floodplain waters. We derive a mathematical model and discuss a generalized collage method for recovering diffusion parameters present in this model. Theoretical and numerical particulars are discussed and results are presented.

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The Monge-Kantorovich Metric in Applications

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The Monge-Kantorovich metric is derived from the Kantorivich's linear relaxation of Monge's mass transportation problem. As such, it has connections with many different areas of analysis. For the purposes of this talk, however, it is mainly useful as a particularly nice metric between probability measures on a metric space.

Let X be a compact metric space and $\mathscr{P}(X)$ be the space of Borel probability measures on X. There are many different metrics one can place on $\mathscr{P}(X)$, however, it is often desirable to have the distance between distributions linked in some way with the underlying metric on X. The MK metric does this through its connection with mass transportation. More specifically, if we let $\mathscr{L}(X) = \{f : X \to \mathbb{R} : |f(x) - f(y)| \leq d(x,y)\}$ then for $\mu, \nu \in \mathscr{P}(X)$ we have that

$$d_{MK}(\mu,\nu) = \sup\left\{ \int_X f \, d(\mu - \nu) : f \in \mathscr{L}(X) \right\}. \tag{1}$$

For instance, $d_{MK}(\delta_x, \delta_y) = d(x,y)$ if δ_x, δ_y are point masses at $x, y \in X$.

In practical computations the MK metric (1) is defined on a finite discrete space, usually modeled as a graph G, and the integrals become sums. In this setting, computing (1) is a linear program and thus there are many well-known approaches. However, in applications it is often desirable to have linear time or near-linear time algorithms for this computation.

In this talk, we will discuss computational approaches to computing the MK distance in applications. Our applications will focus on image matching and recognition. One application is to content-based image retrieval, in which case linear time algorithms are essential. The other application is an insect identification problem, specifically identifying and counting pest mites in images from apple orchards.

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Numerical Solution of 3D Vector Tomography Problem Using a Singular Value Decomposition.

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In this talk the normal Radon transform operator acting on a potential vector field on the unit ball is considered. The normal Radon transform of vector field $\mathbf{w} = (w_1, w_2, w_3)$ is defined by formula

$$\left[\mathscr{R}^{\perp}\mathbf{w}\right](\xi, s) = \int\limits_{P_{\xi,s}} \left(w_1\xi^1 + w_2\xi^2 + w_3\xi^3\right) \mathrm{d}u\mathrm{d}v, \tag{1}$$

here $P_{\xi,s}$ is a plane, which is orthogonal to the direction ξ and the distance between the plane and the origin of coordinates is equal to $|s|$. Coordinates of the local coordinate system on plane $P_{\xi,s}$ are u, v. Our goal is to construct the singular value decomposition of the operator.

The orthogonal bases in the initial space are constructed using harmonic and Jacobi polynomials. A connection between the normal Radon transform of the potential vector field and the Radon transform of the potential, which is equal to zero on domain boundary, is obtained by the author of this paper. Using this connection and a result from [1] the author showed that the orthogonal bases in the image space are constructed using harmonic and Gegenbauer polynomials.

The inversion formula is derived on the basis of the obtained singular value decomposition of the normal Radon transform operator. This algorithm was used to solve a 3D vector tomography problem, namely for reconstruction of a potential part of a 3D vector field if its normal Radon transform is known. For this a truncated singular value decomposition is used. Numerical tests for data sets with different noise levels of smooth and discontinuous fields show the validity of the approach.

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Parameter and State Range Reduction for ODE Models using Monotonic Linear Multistep Discretizations

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We consider the problem of fitting an ODE model to time series data. This process traditionally involves finding the best parameter values with respect to some error expression. These methods can be deterministic or probabilistic and an excellent comparison of a variety of methods can be found in [1]. While these techniques tend to be computationally efficient, they can easily fail to converge, or converge to a poor solution.

An alternative to these techniques is to assume that each parameter is contained in some a priori range and use interval methods to reduce these ranges [2, 3]. This is typically accomplished by integrating using a validated solver, comparing the derived solution with the observed data and removing inconsistent regions of parameter space. These methods provide a tight enclosure of the true parameter values, but can be computationally expensive.

Our work is an extension of the more efficient interval method published in [4]. Linear multistep methods are used to discretize each equation over a chosen time window. These methods can be written in the form

$$F = -\sum_{i=0}^{s} \alpha_i x^i + h \sum_{i=0}^{s} \beta_i f^i = 0, \tag{1}$$

where x^i and f^i represent the state variable and vector field respectively evaluated at the i-th time step. To be consistent, the resultant interval discretization must enclose the discretization error and we can discard regions of parameter space that fail this condition. This method relies on obtaining monotonicity of F with respect to each parameter to improve efficiency and provide a quick parameter reduction scheme.

In this work, we consider the case in which some state variables are unmeasured. It is reasonable to assume that some variables present in an ODE model are not feasibly measurable and we may have to assume potentially wide initial ranges for these variables. We show that by considering the unmeasured state variables at each time step in equation (1) as additional parameters, we can apply the parameter reduction scheme described above. We describe the required modifications to the original method to accommodate unmeasured variables. These modifications include the development of a new linear multistep discretization, improved performance in the computer implementation of the original algorithm, the ability to handle non-monotonic parameters and the introduction of the *hull consistency test*. We also present some results obtained from sample test systems.

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Regularizing a Volterra Integral Equation of the First Kind

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We consider the inverse problem of solving for the function u, when

$$\int_0^x K(x,t)u(t)\,dt = g(x),\ 0 \le x \le T. \tag{1}$$

Here, the kernel K and the function u are assumed to be exact, but the right hand side g represents observations and T is a fixed number. Equation (1) is a Volterra integral equation of the first kind. We deal with the particular case where g represents a sparse set of measurements at the points $\{x_1,\ldots,x_N\}$ of a fixed grid. The grid-points $x_1 < \ldots < x_N$ are assumed to be known exactly and the measured values g_i are approximations of the functional values $g(x_i)$. Then Eq. (1) may be replaced by

$$\int_0^{x_i} K(x_i,t)u(t)\,dt = g_i,\ i = 1,\ldots,N. \tag{2}$$

This problem occurs in porous media physics as the task of converting centrifuge data into a capillary pressure function. Deriving the capillary function involves the unstable process of inverting a linear smoothing operator. The operator for this particular problem has no bounded inverse.

We show that a regularized solution of the inverse problem is obtained by constraining the solution space to monotone and convex functions. These constraints, which satisfy certain physical constraints, may be expressed in the form of linear inequalities. We then arrive at a solution which approximates the measured values as closely as possible, where the deviation is defined by a suitable norm.

We present numerical experiments which compare different discretization schemes, and results for real experimental data.

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B-Spline Slice-by-Slice Solution of a 3D-Vector Tomography Problem.

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In this paper the 3D-vector tomography problem is considered in the following formulation. Let a bounded domain in R^3 be filled by a medium without refraction (probing rays permeate along straight lines). In the domain some vector field v is given. It is required to find this field by its known ray transform.

We consider R^3 as the Euclidean vector space with the standard scalar product $\langle\cdot,\cdot\rangle$ and norm $|\cdot|$. The ray transform $\mathscr{I}$ on R^3 maps a vector field $v=(v_j)$ to the function $[\mathscr{I}v]$ on the manifold of oriented lines $l=\{x+t\xi \mid x,\xi\in R^3,\ |\xi|=1,\ \langle x,\xi\rangle=0,\ t\in R\}$ by the formula

$$[\mathscr{I}v](x,\xi)=\sum_{j=1}^{3}\int_{-\infty}^{\infty}\xi_j v_j(x+t\xi)\,dt.$$

The operator $\mathscr{I}$ possesses a non-trivial kernel consisting of potential vector fields with vanishing potentials on the boundary [1]. Therefore only the solenoidal part ${}^s v$ of the field v can be recovered from $[\mathscr{I}v]$.

The problem is overdetermined in dimension, because we try to recover functions ${}^s v_j(x)$, where $x\in R^3$, from the function $[\mathscr{I}v]$ on the four-dimensional manifold of oriented lines (variables x,ξ have the dimension 6 in total, but there are two conditions: $|\xi|=1,\ \langle x,\xi\rangle=0$). Therefore it is natural to pose the problem of recovering ${}^s v$ from incomplete data $[\mathscr{I}v]|_{M^3}$, where M^3 is some three-dimensional submanifold of the manifold of oriented lines.

There are solution algorithms (see [2]) based on the inversion formulas from [3], in which the problem of recovering a solenoidal part of a vector field on R^3 from ray transforms known over all lines parallel to one of the coordinate planes is considered. Two different coordinate planes are sufficient for the uniqueness (2P-problem), but three coordinate planes are needed for the stable reconstruction of a solenoidal part of vector field (3P-problem).

In this talk we propose algorithm of solving of the problem of recovery of a solenoidal part of vector field, which is given in the unit ball. The solution algorithm is based on the least squares method where we use a finite basis consisting of B-splines as basis function. In that sense the method can be seen as a projection method for minimizing an L_2-data fitting term.

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Designing a Search Grid for Parameter Estimation Using Sensitivity Analysis

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When faced with inverse problem solving to retrieve the model parameters corresponding to a given set of observations, the question of which optimization algorithm to use often arises. Many iterative optimization algorithms, such as particle swarm optimization and simplex simulated annealing, are available and have been succesfully employed in the past. However, when dealing with nonlinear models, describing complex phenomena, an iterative approach often gets stuck in local optima, even when strategies to escape these local optima are built in. Furthermore, it often takes a large number of model evaluations to arrive at a good solution. An alternative is to perform an exhaustive grid search over all possible parameter combinations. Nevertheless, when continuous parameters are at stake or a model run is time consuming, a limited number of grid points in the parameter search space is chosen [1]. When 100 grid points, and therefore 100 model evaluations, in the parameter search space are allowed to parameterize two parameters a and b, a naive solution to how to construct the search grid would be to make combinations with ten points uniformly distributed over the range for both parameters. However, such a regular grid is rarely optimal.

We propose an optimized grid design based on the results of a sensitivity analysis. Sensitivity analysis has long proven its use in model building, since often model parameters are uncertain, especially when modeling complex natural systems [2]. It provides model builders with useful insights into the level of uncertainty contributed by each parameter, which can be important for research prioritization and reducing the model complexity by filtering out parameters that have a minor effect on the model outcome. In this work, the ratio of the sensitivity of the parameters a and b is chosen as a heuristic to allocate the 100 grid points over the search space. This approach on average entails a smaller prediction error than when making use of a regular search grid. Further, the approach can be extended to different kinds of models (stochastic models, cellular automaton-based models,...), more parameters and various types of sensitivity measures can be used.

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The Inverse Problem of Fractal Potential Flows

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Fractal Potential Flows have been reasoned to provide an explicit model for the intermittent interaction of eddies [3], relevant to the evolution towards the extremal case of Fully Developed Turbulence. This approach is related in spirit to Chaotic Advection, a dynamical systems approach to mixing [2, 5, 1]. Considering the direct analogy between the celebrated invariant measure of IFS and the invariant flow of this theory via an isometric isomorphism [3], in our talk we reformulate the inverse problem of IFS [4] within the setting of fractal potentials, with the purpose of approximatively modelling the observed interaction of a finite system of eddies. This reformulation is also crucial to measuring the effectiveness of the model in approximating experimental data.

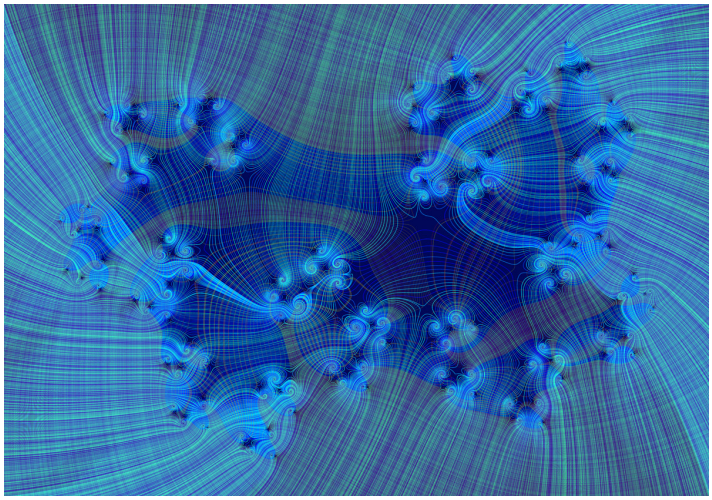

Figure 1: Evolving streamlines and equipotential lines.

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Fourier Transforms of Measure-Valued Images, Self-Similarity and the Inverse Problem

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In [2], a complete metric space (Y, d_Y) of measure-valued images $\mu : [0,1]^n \to \mathscr{M}(R_g)$ was constructed. Here, $\mathscr{M}(R_g)$ is the set of Borel probability measures supported on the *greyscale range* $R_g \subset \mathbf{R}$ (or $\mathbf{R}^m$). A primary motivation for this and other related constructions [5] is that there are situations in image processing in which it is useful to consider the greyscale value of an image u at a point x as a random variable that can assume a range of values $R_g \subset \mathbf{R}$, as opposed to a single value (or set of values, in the case of a vector-valued image, e.g., RGB color image, hyperspectral satellite images of the earth).

A measure-valued representation of images may also be useful in the analysis and implementation of various nonlocal image processing schemes, where the greyscale value of an image $u(x)$ is modified according to the values of the image $u(y_k)$ at points y_k that lie elsewhere in the image and not necessarily close to x. Two such nonlocal schemes examined in [2] using measure-valued representations were (i) *nonlocal means denoising* [1] and (ii) *fractal image coding* [3].

In [2], a fractal transform operator was also constructed over the space (Y, d_Y). For a $\mu \in Y$, the action of a fractal transform $T : Y \to Y$ is to construct N spatially contracted and range-modified copies of μ and recombine them to produce a new element $\nu = T\mu \in Y$. Under suitable conditions T is contractive in (Y, d_Y), implying the existence of a fixed point measure-valued function $\bar{\mu} = T\bar{\mu}$.

The purpose of this paper is to show how Fourier transforms of measure-valued image functions may be defined as complex-valued measures on the greyscale range R_g. We also show that a fractal transform operator T on (Y, d_Y) induces a mapping M on the space $(\mathscr{F}, d_{\mathscr{F}})$ of Fourier transforms. In the case that T is contractive on (Y, d_Y), it follows that M is contractive on $(\mathscr{F}, d_{\mathscr{F}})$. This sets up the possibility of solving inverse problems in the space $(\mathscr{F}, d_{\mathscr{F}})$: Given a Fourier transform $U(\omega)$, find a contractive operator M with fixed point $\bar{U}(\omega)$ which approximates $U(\omega)$ to a prescribed accuracy. Such a method of solving inverse problems in the Fourier domain has been performed for standard image functions [4].

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Denoising of Hyperspectral Images: An Examination of Different Approaches

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Briefly, hyperspectral images (HI) are "data cubes" that contain a collection of images taken at different wavelengths. They are usually taken by a hyperspectral camera and may contain from tens to hundreds of frequency bands depending on the spectral resolution of the camera's sensor. The sensor measures the reflectance values of different wavelengths at each pixel location, which is a measure of the ratio of reflected energy to incident energy. Reflectance is important since different materials exhibit different spectral "fingerprints", so that by taking a look at the spectrum (entire set of reflectances) at a pixel, it is possible to determine the composition/nature of material represented by that pixel. This characteristic makes HI useful for a wide range of applications such as agriculture, mineralogy, physics and surveillance.

As with any image, HI are also prone to be contaminated with noise. Therefore, reconstruction techniques are desirable in order to recover good approximations of the original noise-free hyperspectral data. In this study, we compare four different approaches that address the inverse problem when HI are contaminated with white Gaussian noise. The main difference between these methods is how they process the hyperspectral image, i.e., if they treat the hyperspectral data as a whole, as a collection of frequency bands (often referred to as "channels"), as a set of spectra, or as both a collection of frequency bands and spectra.

In the first approach, we consider HI as collections of spectra. This method allows us to perform either filtering (e.g., wavelet) or regularization (e.g., sparsity) in the spectral domain. In particular, given that the spectra have a sparse representation in a certain domain, we can solve the following sparse approximation problem at each pixel independently:

$$\min_c \left\{ \frac{1}{2}\|D(c)-y\|^2 + \lambda\|c\|_1 \right\}, \tag{1}$$

where y is a noisy spectrum, D is a transformation matrix (e.g., wavelet, DCT, Fourier, etc.), and c is the set of coefficients that are to be recovered.

As for the second approach, we view HI as sets of frequency bands or "channels". In this case, we carry out the regularization in the spatial domain by using the standard channel-by-channel Total Variation (TV) denoising. For each band independently, the following problem is solved:

$$\min_z \left\{ \frac{\delta}{2}\|z-y\|^2 + \|z\|_{TV} \right\}, \tag{2}$$

where $\|\cdot\|_{TV}$ is the total variation norm and y is the noisy band or "channel". Along these lines, for the third approach, a formulation of vectorial TV denoising (e.g., Bresson and Chan's vectorial TV), allows us to denoise the entire hyperspectral image at once. In this case, HI are viewed as a whole.

Finally, for the fourth approach, HI are seen as both collections of spectra and frequency bands. This method involves a combination of the first two approaches, therefore, the denoising is carried out by regularizing in the spatial domain, and by either filtering or regularizing in the spectral domain. This inverse problem can be solved by algorithms such as the Alternating Direction Method of Multipliers (ADMM) and Split Bregman.

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Regularization Approach for Abel Transform Based Image Reconstruction by a Single Radiograph

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The purpose of hydrodynamics experiments is to characterize the state of matter subjected to powerful shocks under the effect of explosives. For axially symmetric objects, only a single radiograph is taken using fan-beam X-rays with a radiographic axis perpendicular to the symmetric axis of the object. To reconstruct the varying density of object leads to Abel transform inversion. In the discrete setting, we formulate the Abel transform as a matrix $A \in R^{m\times n}$, and the object radial density as $\rho \in R^n$. The radiograph process can be characterized by the equation:

$$\mathbf{d} = KA\rho + \mathbf{n}. \tag{1}$$

Here $\mathbf{d}$ denotes the measured data, K and $\mathbf{n}$ respectively represent the blurring kernel and the noise caused by the recording system. To solve ρ from Eq.(1), the contemporary methods ([1, 2]) make the assumption that the density is piecewise constant or linear and the X-rays are parallel. From a practical point of view, this is quite a restrictive approximation. Based on fan-beam X-rays, we propose the high-order total variation regularization model:

$$\min_{\rho}\left\{\mathscr{E}(\rho) = \mu_1\|\nabla\rho\|_1 + \mu_2\|\Delta\rho\|_1 + \frac{1}{2}\|KA\rho - \mathbf{d}\|_2^2\right\}, \tag{2}$$

where Δ is the discrete Laplacian operator, μ_1 and μ_2 are regularization parameters. The optimization problem is solved using the augmented Lagrangian method. We compare our model with other potential regularization techniques, like TV, TGV, LLT. The numerical tests show that the proposed model has advantages on staircasing reduction, density level preservation, CPU time cost and SNR improvement (See Fig. 1, 2).

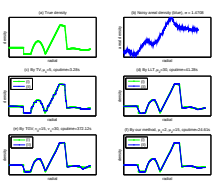

Figure 1: Abel inversion

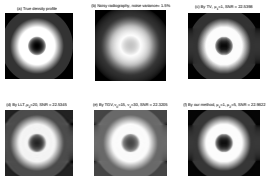

Figure 2: Tomographic reconstruction

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Inverse Problems for Delay Differential Equations Using the Collage Theorem

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Recent research has established a solution framework for differential equations inverse problems via the Collage Theorem. This theorem first proved useful in fractal imaging and is a relatively simple consequence of Banach's Fixed Point Theorem. In an appropriate setting, the solution framework allows us to solve for the unknown parameters of an ODE system by minimizing the $\mathscr{L}^2$ collage distance between a given target solution, which may be the interpolation of observational data, and its image under the associated Picard operator integral mapping, which can be shown to be contractive on a suitable complete metric space.

In our current work, we have developed a similar framework for delay ODE inverse problems, which may involve either discrete (additive) delays, distributed (integral) delays, or both. Such terms introduce a dependence on past time states in the system, which affects the conditions for the boundedness and contractivity of the associated integral mapping.

I will begin this talk by presenting the theory for the mathematical framework. A numerical example with simulated data will follow, with the goal of showing how the theory is implemented and the computational issues that can arise in practice. I will also discuss future applications to a model problem for pollution feedback effects in a human-environmental system.

This is joint research with C. Bauch and H. Kunze, Mathematics and Statistics, University of Guelph.

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Canada-China Session on Applied Dynamic Systems (SS-ADS)

Organizers:
Yuming Chen (Wilfrid Laurier University)
Fengqin Zhang (Yuncheng University)
Xingfu Zou (Western University)

The theory of dynamical systems describes qualitative and quantitative features of solutions of nonlinear systems, typically modelling processes which evolve over time. Its application areas are diverse and multidisciplinary, including biology, physics, finance, industrial mathematics, and engineering. This session will provide a platform for researchers from Canada and China to exchange their latest progress in applied dynamical systems. The significant goal is to facilitate interaction and discussion, which will seed new research projects.

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Advances in Impulsive Differential Equations

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Many dynamical systems have an impulsive dynamical behavior due to abrupt changes at certain instants during the evolution process. The mathematical description of these phenomena leads to impulsive differential equations. Impulsive differential equation is one of the main tools to study the dynamics of processes in which sudden changes occur. The theory of impulsive differential equation has recently received considerable attention. Some classical tools such as fixed-point theorems in cones and the method of upper and lower solutions with monotone iterative technique have been widely used to study impulsive differential equations. In the last few years, a new approach via critical point theory and variational methods is proved to be novel and very effective in studying the existence of solutions for impulsive differential equation possessing a variational structure under certain boundary condition.

This talk gives an overview of some results obtained in recent years in the exis- tence of solutions to impulsive problems via variational methods and critical point theory. In particular, we discuss the solvability of a class of impulsive damped vibration problems via variational methods and critical point theory. Our results are more general. The obtained results are also valid and new even if the impulsive damped vibration problem is reduced to impulsive Hamiltonian system and Hamiltonian system. Finally, some corollaries are presented and examples are given to illustrate the main results.

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A positivity preserving semi-implicit numerical method for a highly nonlinear diffusion-taxis-reaction model

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The following highly nonlinear quasilinear diffusion-reaction system has been proposed in [1] to describe interacting volume filling, interface propagation and chemotaxis phenomena in biological populations:

$$\begin{cases} \partial_t S &= d\partial_{xx} S - F(S,M) \\ \partial_t M &= \partial_x \left(D(M)\partial_x M\right) + \partial_x \left(\chi(M)\partial_x S\right) + G(S,M) \end{cases} \tag{1}$$

with diffusion nonlinearities

$$D(M) = \delta_1 \frac{M^b}{(1-M)^a}, \quad \chi(M) = \delta_2 M^d (1-M)^c, \tag{2}$$

and reaction nonlinearities

$$F(S,M) = \frac{k_1 SM}{k_2 + S}, \quad G(S,M) = \frac{k_3 SM}{k_2 + S} M^\alpha (1-M)^\beta, \tag{3}$$

subject to suitable initial and boundary conditions, and restrictions on the exponents of the nonlinearities that will be made precise in the talk. Here M describes the population density and S the concentration of a nutrient.

In the talk, we will first give a review of the analytical well-posednessresults concerning this model, which were derived in [1], and then present a semi-implicit numerical method for its simulation. The method is based on a Finite Volume discretization in space and a non-local (in time) presentation of the nonlinearities. This method is a cross-diffusion extension of the one developed in [2] for a related but simpler model. We will show that the numerical method is well-posed and preserves positivity. The convergence of the method, and its ability to describe interface propagation phenomena is demonstrated in a numerical grid refinement study.

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Epidemic dynamics on semi-directed complex networks

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Modeling infectious diseases on complex networks has recently attracted tremendous interest among the public health modelers. This approach assumes that a population can be represented by complex networks in which the nodes represent individuals and the links represent various interactions among those individuals. Pastor, et. al. [1] and Wang, et. al. [2, 3] studied the symmetric and asymmetric transmissions of the epidemic based on the undirected networks and directed networks, respectively. In the real world both symmetric and asymmetric contacts can occur in the same contact network, so called semi-directed complex network. In this talk an SIS model for epidemic spreading on semi-directed networks is established, which can be used to examine and compare the impact of undirected and directed contacts on disease spread. The model is analyzed for the case of uncorrelated semi-directed networks, and the basic reproduction number R_0 is obtained analytically. We verify that the R_0 contains the outbreak threshold on undirected networks [1] and directed networks [2, 3] as special cases. It is proved that if $R_0 < 1$ then the disease-free equilibrium is globally asymptotically stable, otherwise the disease-free equilibrium is unstable and the unique endemic equilibrium exists, which is globally asymptotically stable. Finally the numerical simulations holds for these analytical results are given.

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Controllability of second order impulsive functional differential systems with infinite delay in Banach spaces

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In this paper, we study the approximate and exact controllability of second order impulsive functional differential systems with infinite delay of the form

$$\begin{aligned} &x''(t) = Ax(t) + Bu(t) + f(t, x_t, x_t'), \ \ t \in J, \ \ t \neq t_k, \\ &\Delta x|_{t=t_k} = I_k^1(x(t_k)), \ \ k = 1, \cdots, m, \\ &\Delta x'|_{t=t_k} = I_k^2(x'(t_k^+)), \ \ k = 1, \cdots, m, \\ &x_0 = \phi \in \mathscr{B}, \ \ x_0' = \varphi \in \mathscr{B}, \end{aligned} \tag{1}$$

where $J = [0, b]$, the state $x(\cdot)$ takes values in Banach space X with the norm $\|\cdot\|$, $u(\cdot) \in L^2(J, U)$ is the control function, U is a Banach space, A is the infinitesimal generator of a strongly continuous cosine family $\{C(t) : t \in R\}$ on X, $B : U \to X$ is a bounded linear operator. $0 = t_0 < t_1 < \cdots < t_m < t_{m+1} = b$, $\Delta x|_{t=t_k} = x(t_k^+) - x(t_k^-)$, $\Delta x'|_{t=t_k} = x'(t_k^+) - x'(t_k^-)$, and $I_k^j : X \to X, \ j = 1, 2, \ f : J \times \mathscr{B} \times \mathscr{B} \to X$ are appropriate continuous functions to be specified later. The histories $x_t, x_t' : (-\infty, 0] \to X, \ x_t(\theta) = x(t + \theta), \ x_t'(\theta) = x'(t + \theta), \ \theta \leq 0$, belong to some abstract phase space $\mathscr{B}$ defined axiomatically. Sufficient conditions are established for each of these types of controllability. The results are obtained by using the theory of strong continuous cosine families of bounded linear operators and the contraction mapping principle. Particularly, the compactness of the cosine operator is not needed in this paper. An example is presented to illustrate the obtained conclusions. Our results extend those of Mahmudov et al. [1], Sakthivel et al. [2], Park et al. [3] and Chalishajar et al. [4].

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Using Lyapunov Functions to Construct Lyapunov Functionals

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Many epidemic models are based on ordinary differential equations (ODEs) and can be written as

$$x'(t) = f(x(t)). \tag{1}$$

Standard analysis includes calculating the basic reproduction number $\mathscr{R}_0$. Models often exhibit threshold behaviour where there is a disease-free equilibrium that is globally asymptotically stable for $\mathscr{R}_0 < 1$ and an endemic equilibrium that is globally asymptotically stable for $\mathscr{R}_0 > 1$. Since Korobeinikov's paper in 2004 [1], the case where $\mathscr{R}_0 > 1$ has been resolved for many ODE models through the use of Lyapunov functions based on the Volterra function

$$g(x) = x - 1 - \ln x. \tag{2}$$

Other models include delay to better describe certain biological processes. These systems can be written as

$$x'(t) = f(x(t), x(t-\tau)) \tag{3}$$

or, more generally,

$$x'(t) = f(x_t), \tag{4}$$

where $x_t : [-\tau, 0] \to R^n$ for some $\tau > 0$. In [2], a Lyapunov functional (based on the Volterra function g) was used to resolve the global stability for two disease models with delay for the case where $\mathscr{R}_0 > 1$. Since then a similar approach has been used to prove the classical threshold behaviour for many disease models that involve delay. In reviewing the many examples, it becomes clear that the Lyapunov functional for the delay equation is very strongly related to the Lyapunov function that works for the corresponding ODE.

In this work, we analyze the connection between the Lyapunov functional that works for Equation (4) and the Lyapunov function that works for the corresponding ODE. Using careful mathematical analysis, we obtain a test that allows one to classify, a priori, the terms that can incorporate delay without affecting the global asymptotic behaviour of the system.

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Agent-Based Modelling for Disease Dynamics in-silico Populations

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Modelling and computational approaches provide powerful tools in the study of disease dynamics at both the micro and macro levels. Recent analytical developments, coupled with advances in information and communications technologies, have opened up novel vistas and presented new challenges in mathematical epidemiology. Key challenges involve ways to deal with the collective dynamics of heterogeneous ensembles of individuals, and to analyze data that are less coarse and more complex. The evolution of dynamic modelling is typified by the agent-based modelling (ABM) paradigm, a lattice-distributed collection of autonomous decision-making entities (i.e., agents), the interactions of which unveil the dynamics and emergent properties of an infectious disease outbreak. The flexibility of ABMs permits an effective representation of the complementary interactions between individuals characterized by localized properties and populations at a global level. In this talk, we discuss the importance of ABMs in understanding epidemic spread, and identifying optimal intervention strategies in different population settings with distinct demographic characteristics.

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The Impact of a Single-strain Flu Vaccine on the Dynamics of a Two-strain influenza

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Vaccination is considered one of the most effective control measures for influenza. However, when a virus mutates and multi-strains appear in a population, implementing a vaccine for one strain may affect the spread of the other strains. In this paper, we propose a two-strain model and investigate the effects of a single-strain vaccine on the dynamics of this two-strain model. The global dynamics of the model are completely determined through suitable Lyapunov functions. We show that if the basic reproduction number is less than one, then both strains die out; but when the number is larger than one, one or both of the strains become endemic depending on the parameter values. The theoretical results provide some useful information on the impact of the vaccination rate of this single-vaccine for one strain on the dynamics of the two strains.

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Codimension-1 sliding bifurcations of Filippov pest growth model with threshold policy

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The Filippov system is proposed to describe the stage structured non-smooth pest growth with threshold policy control (TPC). We consider three TPC methods represented by either the density of the juveniles, the density of the adults, or the total density of both juveniles and adults being chosen as an index for decisions on when to implement chemical control strategies. The proposed Filippov system with total density as the index has at most three pieces of sliding segments, while the density of juveniles or adults guided switching systems can only have at most two pieces of sliding segments. The existence of multiple sliding segments and pseudo-equilibria result in rich sliding mode bifurcations and local sliding bifurcations including boundary node (boundary focus, or boundary saddle) and tangency bifurcations. As the threshold density varies we examine the global sliding bifurcations for the proposed Filippov system, and the interesting bifurcations occur sequentially: touching $\rightarrow$ buckling$\rightarrow$ crossing $\rightarrow$ sliding homoclinic orbit to a pseudo-saddle$\rightarrow$ crossing $\rightarrow$ touching bifurcations. Further, bifurcation of a homoclinic orbit to a pseudo-saddle with a figure of eight shape, to a pseudo-saddle-node or to a standard saddle-node have been observed for some parameter sets.

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Mathematical Model of Anaerobic Digestion in a Chemostat: Effects of Syntrophy and Inhibition

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Anaerobic digestion is a complex naturally occurring process during which organic matter is broken down to biogas and various byproducts in an oxygen-free environment. It is used for waste and wastewater treatment and for production of biogas, especially methane. A system of differential equations modelling the interaction of microbial populations in a chemostat is used to describe three of the four main stages of anaerobic digestion: acidogenesis, acetogenesis, and methanogenesis. To examine the effects of the various interactions and inhibitions, we first study an inhibition-free model and obtain results for global stability using differential inequalities together with conservation laws. These results are compared with the predictions for the model with inhibition. In particular, inhibition introduces regions of bistability and stabilizes some equilibria.

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Modeling effects of environmental contamination and volunteers on hospital infections in China

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In this talk I shall present deterministic and stochastic mathematical models with indirect transmission via free living bacteria in the environment to investigate the roles that environmental contamination and the presence of volunteers played in the dynamics of hospital infections in China. Semi-stochastic simulation was used to estimate some of the parameters by fitting the observed data and investigating the impacts of interventions such as cleaning, hand hygiene and isolation of admitted MRSA (Methicillin-resistant *Staphylococcus aureus*) patients on mean prevalence of infection. Numerical simulations show that environmental contamination is a threat to hospital infection and free-living bacteria in the environment can promote transmission and initiate infection even if an infection has died out among HCWs (health-care workers) and patients. Sensitivity analysis indicates that a contaminated environment and volunteers contribute substantially to MRSA transmission in hospital infections. Hand hygiene of volunteers and cleaning are more effective in reducing the mean prevalence of colonized patients than isolation of newly admitted MRSA- positive patients and hand hygiene of HCWs. Hence volunteers, a cadre of semi-professional nurses, are beneficial to both disease control and supplementary treatment of HCWs if they are well trained [1, 2].

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Global stability of some epidemic models with age structure

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Abstract

Infection age is an important factor affecting the transmission of infectious diseases. In this talk, we consider some epidemic models with infection age, which is described by a mixed system of ordinary differential equations and partial differential equations. The expression of the basic reproduction number $\mathscr{R}_0$ is obtained. If $\mathscr{R}_0 \leq 1$ then the model only has the disease-free equilibrium, while if $\mathscr{R}_0 > 1$ then besides the disease-free equilibrium the model also has an endemic equilibrium. Moreover, if $\mathscr{R}_0 < 1$ then the disease-free equilibrium is globally asymptotically stable otherwise it is unstable; if $\mathscr{R}_0 > 1$ then the endemic equilibrium is globally asymptotically stable. The local stability is established through linearization. The global stability of the disease-free equilibrium is shown by applying the fluctuation lemma and that of the endemic equilibrium is proved by employing Lyapunov functionals. The theoretical results are illustrated with numerical simulations.

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Dirichlet problem of delayed reaction-diffusion equations involving semi-infinite intervals

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We derive a nonlocal delayed reaction-diffusion equation in a semi-infinite interval which describes the single species population with two age classes and a fixed maturation period living in a spatially semi-infinite environment. To overcome the difficulty in describing the global dynamics due to the non-compactness and asymmetry of the spatial domain, we establish *a priori* estimate for nontrivial solutions after describing the delicate asymptotic properties of the nonlocal delayed effect and the diffusion operator. The estimate enables us to show the permanence of nontrivial solution and the existence of heterogeneous steady state in the case of Dirichlet boundary conditions. Thus, we can employ standard dynamical system theoretical arguments to establish the global attractivity of the heterogeneous steady state.

Advanced Numerical Methods for PDEs and Applications (SS-ANMPDE)

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Peter A. Forsyth (University of Waterloo)
Dong Liang (York University)

This special session aims to provide a platform to present recent developments in numerical methods for PDEs, enable in-depth discussions on a variety of computational efforts for solving problems arising in areas of science, engineering, finance, etc, and foster the interdisciplinary culture required to meet recent challenges in scientific computation. Example applications include optimal trade execution, electromagnetics, environmental modelling, and wind-energy computation.

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ML-α-Deconvolution model in a bounded domain with a vertical regularization

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In this talk, we consider the deconvolution modified Leray alpha (ML-α-deconvolution) model with fractional filter acting only in one variable

$$\mathbb{A}_{3,\theta} := I + \alpha_3^{2\theta}(-\partial_3)^{2\theta}, \quad 0 \leq \theta \leq 1. \tag{1}$$

This filter is less memory consuming than the classical one [2]. Moreover, there is no need to introduce artificial boundary conditions for Helmholtz operator. It was shown in [1] that the Large Eddy Simulation models which are derived by using $\mathbb{A}_{3,\theta}$ for any $\theta > \frac{1}{2}$, are well-posed. Motivated by this work [1], we study the global existence and uniqueness of solutions to the vertical ML-α-deconvolution model on a bounded product domain of the type $D = \Omega \times (-\pi, \pi)$, where Ω is a smooth domain, with homogeneous Dirichlet boundary conditions on the lateral boundary $\partial\Omega \times (-\pi, \pi)$, and with periodic boundary conditions in the vertical variable. To present the model, we define the vertical Nth Van Cittert deconvolution operator by

$$D_{N,\theta} = \sum_{i=0}^{N} (I - \mathbb{A}_{3,\theta}^{-1})^i. \tag{2}$$

The vertical ML-α-deconvolution model is then defined, for some fixed $\theta > 0$, with a filtering radius $\alpha_3 > 0$, a kinematic viscosity $\nu > 0$, a deconvolution order $N \geq 0$, and an initial velocity v_0 as follows,

$$\begin{aligned} \partial_t v + (v \cdot \nabla) D_{N,\theta}(\bar{v}) - \nu \Delta v + \nabla p &= f, \\ \nabla \cdot v &= 0, \\ v(0) &= v_0 = 0, \end{aligned} \tag{3}$$

where v and p are the velocity and the pressure, $\bar{v} = \mathbb{A}_{3,\theta}^{-1}(v)$ is the smoothed velocity, and f is a forcing term. In order to state our main result, let us define the following spaces:

$$L^2(D) := \left\{ v \in L^2(D)^3, 2\pi\text{-periodic in } x_3 \right\}, \tag{4}$$

$$H := \left\{ v \in L^2(D), \text{ such that } \nabla \cdot v = 0 \text{ and } v \cdot n = 0 \text{ on } \partial\Omega \times (-\pi, \pi) \right\}, \tag{5}$$

$$V := \left\{ v \in H, \text{ such that } \nabla v \in L^2(D) \text{ and } v = 0 \text{ on } \partial\Omega \times (-\pi, \pi) \right\}. \tag{6}$$

Our main result is the following.

Theorem 1. *Assume $f \in L^2(0,T;H)$ and $v_0 \in H$. let $0 \leq N < \infty$ be a given and fixed number and let $\theta > \frac{1}{2}$. Then problem (3) has a unique regular weak solution.*

This result holds also true on the whole space $\mathbb{R}^3$ and on the torus $\mathbb{T}_3$. Other α models, with partial filter, will be reported in a forthcoming paper.

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A Truncated FCI Approach Motivated from the Mathematics of Complexity for Solving the Electronic and Nuclear Schrödinger Equation

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Few electronic structure and nuclear structure (nuclear physics) methods are able to obtain a given desired accuracy for solving the Schrödinger equation. The most obvious method for reliably achieving a given desired accuracy is the full-configuration interaction (Full-CI) method. However, Full-CI is very computationally expensive (exponential scaling) and as such is rarely useful other than for benchmarking calculations. Full-CI is a method that would work for any arbitrary Hamiltonian. Thus, Full-CI does not take advantage of the inherent smoothness associated with the solutions to the Hamiltonians appropriate for electronic structure calculations or for nuclear structure calculations. Results from Griebel and others[1-4] in the mathematics of complexity literature show that if the analytic solutions to a given Schrödinger equation have mixed bound derivatives then it is possible to obtain Full-CI accuracy with polynomial scaling (at least in the large basis set limit). The approach involves selecting a subset of the solutions used in the Full-CI method (typically a subset of all possible Hartree-Fock solutions). The theorems indicate which solutions to include based on the number of nodes in each solution. We refer to this approach as the GK-CI method.[5] This truncation of the Full-CI method does not require any physical intuition of orbitals (e.g. the Hartree-Fock solutions) and is not constructed from the typical excitation-hierarchy approach. In this presentation I will explain the method as well as provide preliminary results from both electronic structure and nuclear structure calculations.

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An numerical impulse control PDE approach for continuous time optimal portfolio allocation under jump-diffusions

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We present efficient PDE methods for continuous time mean-variance portfolio allocation problems when the underlying risky asset follows a jump-diffusion. The standard formulation of mean-variance optimal portfolio allocation problems, where the total wealth is the underlying stochastic process, gives rise to a one-dimensional nonlinear HJB PIDE with the control present in the integrand of the jump term, and thus, very challenging to solve efficiently. We formulate the asset allocation problem as a two-dimensional impulse control problem, one dimension for each asset in the portfolio, namely the bond and the stock. We then develop a numerical scheme based on a semi-Lagrangian type method, which we show to be monotone, consistent, and stable. Hence, the numerical solution is guaranteed to converge to the unique viscosity solutions of the corresponding HJB PIDE. We also discuss realistic financial modeling, such as different borrowing and lending interest rates and transaction costs, as well as realistic constraints on the portfolio, such as maximum limits on borrowing and solvency of the portfolio.

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On the game p-Laplacian on graphs for processing and clustering of high dimensionnal data

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The purpose of this paper is to introduce and to study a new class of non-local normalized p-Laplacian on graphs. These operators interpolate between non local Laplacian and infinity Laplacian on graphs and are obtained as graph discretization of the well known normalized p-Laplacian or game p-Laplacian [1][2]. Then, we study the Dirichlet problem associated to these operators and prove existence and uniqueness of solutions. Finally, we propose to use these operators as a framework for solving many inverse problems in image processing and machine learning.

We consider an undirected weighted graph $G=(V,E,w)$ with a finite set V of vertices and a finite set $E \subset VxV$ of edges. It is associated with a symmetric weight function $w: VxV \to [0,1]$. The weight function represents a similarity measure between two vertices of the graph. According to w, the set of edges can be defined as $E=\{(u,v): w(u,v)>0\}$. Let $A \subset V$ be a set of connected vertices with. We denote by $\partial A=\{u \in A: \exists v \in A^c \ w(u,v)>0\}$ the boundary sets of A. A^c is the complement of A.

We introduce the non-local p-normalized p-Laplacian on graphs as the following:

$$\Delta_{w,\alpha,\beta} f(u) = \alpha \Delta_{w,\infty} f(u) + \beta \Delta_{w,2} f(u) \qquad (1)$$

$$\text{With } \alpha, \beta >= 0, \alpha + \beta = 1$$

$\Delta_{w,\infty} f$ is the non-local infinity Laplacian on graph defined as:

$$\Delta_{w,\infty} f(u) = \frac{1}{2}\left(\max_{v \in V}\left(\sqrt{w(u,v)}\max\left(f(v)-f(u),0\right)\right)+\min_{v \in V}\left(\sqrt{w(u,v)}\min\left(f(v)-f(u),0\right)\right)\right)-f(u)$$

$\Delta_{w,2} f$ is the non-local Laplacian on graph defined as

$$\Delta_{w,2} f(u) = \frac{1}{\sum_{v \in V} w(u,v)}\left(\sum_{v \in V} w(u,v)\left(f(v)-f(u)\right)\right)-f(u)$$

For details about the non-local infinity Laplacian and Laplacian operators see [3][4].

We are interesting to study the following Dirichlet problem: For a given a function $g: \partial A \to R$, our objective is to find a function $f: V \setminus \partial A \to R$, such that $f=g$ on ∂A and f satisfies Partial difference Equation:

$$\Delta_{w,\alpha,\beta} f(u) = 0 \quad on \quad A \qquad (2)$$

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Optimal Trade Execution: Mean Variance or Mean Quadratic Variation?

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Algorithmic trade execution has become a standard technique for institutional market players in recent years, particularly in the equity market where electronic trading is most prevalent. A trade execution algorithm typically seeks to execute a trade decision optimally upon receiving inputs from a human trader.

A common form of optimality criterion seeks to strike a balance between minimizing pricing impact and minimizing timing risk. For example, in the case of selling a large number of shares, a fast liquidation will cause the share price to drop, whereas a slow liquidation will expose the seller to timing risk due to the stochastic nature of the share price.

We compare optimal liquidation policies in continuous time in the presence of trading impact using numerical solutions of Hamilton Jacobi Bellman (HJB) partial differential equations (PDE). In particular, we compare the time-consistent mean-quadratic-variation strategy (Almgren and Chriss) with the time-inconsistent (pre-commitment) mean-variance strategy. The Almgren and Chriss strategy should be viewed as the industry standard.

We show that the two different risk measures lead to very different strategies and liquidation profiles.

In terms of the mean variance efficient frontier, the original Almgren/Chriss strategy is significantly sub-optimal compared to the (pre-commitment) mean-variance strategy.

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Efficient Splitting Characteristic Method for Aerosol Transports in Environment

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Global climate change and warming in atmosphere have been widely recognized. As one of most important constituents, aerosols have a direct radiative forcing by scattering and absorbing solar and infrared radiation in atmosphere, while they have an indirect radiative forcing associated with the changes in cloud properties by decreasing the precipitation efficiency of warm clouds. In these processes, the physical states including the gas and aerosol phases (i.e. gas, liquid and solid) and the composition of aerosols including the aerosol-associated water mass and the multi-components of aerosols are of great signficance. Numerical simulation has been playing a key role in the study of aerosol processes and aerosol concentration distributions in the atmospheric environment prediction and the air quality control.

Aerosol transport model in atmosphere is a complex multi-component system that involves several physical and chemical processes, such as emission, advection, dispersion, deposition and aerosol processes including condensation/evaporation, coagulation and aerosol chemistry, and the area it studies usually covers a large region. In some aerosol transport computational systems, small time steps have to be used in order to ensure the numerical stability of the numerical schemes, which brings a huge cost of computation. It is an important and challenging task to develop efficient numerical algorithm for multi-component aerosol transport predictions.

In this study, we develop the efficient splitting characteristic method for the aerosol transports in environment. We propose the characteristic method to solve the transport process in the spatial dynamical system by combining with the splitting technique. The developed method can efficiently compute the prediction of multi-component aerosol transport dynamics in high-dimensional domains with a large range of aerosol concentrations and for different types of aerosols including aerosols containing sea salt component. Numerical tests show the computational efficiency of the characteristic method comparing with other algorithms such as Runge-Kutta method (RKM). An actual simulation focusing on the sulfate pollution is taken in the domain with a varying wind field near Pittsburgh. Moreover, simulations of multi-component aerosols over a large domain in the southeast of America are studied. The developed algorithm can be applied for the large scale predictions of multi-component aerosol in multi regions and levels in environment.

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Application of Generalized Multiscale Finite Element Method in Multiphase Flow Models

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Many physical processes in science and engineering are described by partial differential equations whose coefficients vary over many length scales. Typical examples may include subsurface flows where the permeability of the porous medium is represented by a high-contrast, heterogeneous coefficient. In recent decades, multiscale methods have been introduced as an effective tool for treating these types of problems. An important component of these types of methods is the independent construction of a set of multiscale basis functions that span a coarse grid solution space. In particular, once a pre-computed set of basis functions is available, a specified global coupling mechanism may be used in order to obtain the associated coarse scale solution. As the fine scale information is imbedded into the basis functions, a coarse grid solution inherits the fine scale effects of the underlying system.

While standard multiscale methods have proven effective for a variety of applications, in this presentation we consider a more recent framework in which the coarse spaces may be systematically enriched to converge to the fine grid solution. The enrichment procedure hinges on the construction of localized spectral problems, where dominant eigenfunctions are used in the construction of the enriched space [2, 3]. This type of spectral enrichment allows for the number basis functions (and the size of the coarse space) to be flexibly chosen such that a desired level of numerical accuracy may be achieved. In this paper we follow the framework of the Generalized Multiscale Finite Element Method (GMsFEM) in which the enriched functions are incorporated into a continuous Galerkin (CG) global formulation in order to obtain approximate pressure solutions.

An advantage of employing a continuous Galerkin multiscale formulation is the relative ease of implementation. However, a well known limitation of CG is that the resulting solution does not satisfy local conservation. In particular, in the cases when it is necessary to couple the resulting fluxes to a transport equation, local conservation is required. We consider the alternative of post-processing a global CG solution in order to obtain the desired conservation. In this presenation, we generalize the procedure offered in [1] in which the authors perform a global solve and subsequent element-based computations to achieve conservation. To test the performance of the proposed method we solve a standard two-phase flow model using a variety of high-contrast permeability coefficients. In all cases, an increase in the dimension of the coarse solution space yields solutions that are shown to more accurately capture the behavior of the fine scale. In particular, the error decline of the elliptic solution (which has been rigorously analyzed in [2]), is directly inherited by the resulting flux values and two-phase saturation solutions.

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Domain Decomposition Techniques for Electromagnetic Scattering from Thin Wires

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We discuss extensions of our recent work [1] concerning approximate solutions of the electric field integral equation applicable to scattering from thin perfectly conducting wires. Integrators applied to the solution of this problem must accommodate two spatial scales: the kernel of the surface integral equation varies on the scale of the wire radius in a neighborhood of its logarithmic singularity where the source and observation points coincide; outside of this region, the kernel varies on the scale of the excitation wavelength. Our algorithm decomposes the computational domain into a series of segments in which we pose separate expansions for the unknown surface current. This approach gives us the flexibility to locally refine the mesh where necessary while not over resolving the solution in other regions of the domain. One significant difficulty arises when observation points lie very near but outside an integration sub-domain; this poses a challenging problem of a well-known nature: the near-singular integration problem. In this talk we address the resolution of this issue and demonstrate our high order algorithms for difficult computational cases.

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(Towards) a multicore adaptive space time method for PDEs

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There is a continuing need to pursue the development, implementation and theoretical analysis of algorithms for the numerical solution of time dependent PDEs particularly suited to today's increasingly complex problems of interest. Moreover, there is an opportunity to study algorithms designed to take advantage of evolving computing hardware - available commodity clusters, hybrid CPU-GPU systems and even desktop machines with 4-24 cores. Such algorithms consist of three modules: (1) a procedure to step forward in time, (2) the computation of a new spatial mesh as required, and (3) the solution of the (physical) PDE on the newly constructed mesh. Moving mesh methods, developed over the last 30 years, have proven to be a robust and efficient choice to track solutions of PDEs which evolve over disparate space and time scales. Domain decomposition (DD) parallelizes a computation by partitioning the spatial domain into subdomains. The solution on each subdomain is computed by individual processors or cores. With appropriate conditions to transmit solution information between cores, the subdomain solutions can be rapidly combined to give a solution to the original problem. The application of DD methods for the physical PDE, step (3) above, is well established. Here we will consider the application of DD to the PDE based mesh generation problem used in the moving mesh method. If time permits we will show how to couple the Revisionist Integral Deferred Correction approach (for small scale parallelism in time) with domain decomposition to give a fully parallel space-time method.

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Multicomponent polymer flooding in two dimensional oil reservoir simulation

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We propose a finite volume method to study the Buckley-Leverett equation with multicomponent polymer flooding in the presence of gravity, The system of equations is given by

$$\begin{aligned} s_t + \nabla \cdot F(s, c_1, c_2, ...c_m, x)) &= 0 \\ (sc_l + a_l(c_l))_t + \nabla \cdot (c_l F(s, c_1, c_2, ...c_m, x)) &= 0, \quad l = 1, 2, ..., m, \end{aligned}$$

where s , c_l are saturation of water and concentration of the polymers respectively and the flux function F is given by $F(s, c_1, c_2, ..., c_m, x) = [v(x) - (\rho_w - \rho_o) g \lambda_o K(x) \hat{y}] f(s, c_1, c_2, ...c_m)$, where ρ_w, ρ_o are the densities of water and oil, g is the acceleration due to gravity and $\hat{y} = [0, 1]$ is the unit vector pointing in the positive y-direction (opposite to gravity), $K(x)$ is the absolute permeability of the rock, $f = \frac{\lambda_w}{\lambda_w + \lambda_o}, \lambda_w(s, c_1, c_2, ...c_m)$ and $\lambda_o(s, c_1, c_2, ..., c_m)$ are mobilities of water and oil respectively. The velocity v which is assumed to be incompressible, is given by $v = -(\lambda_w + \lambda_o) K \nabla p - (\lambda_w \rho_w + \lambda_o \rho_o) g K \hat{y}$.

This problem was studied in [3, 4] numerically in the absence of gravity. In the presence of gravity, the exact Riemann solver for this problem is too complicated due to the fact that we have to deal with a system of $m+1$ variables and the permeability K could be discontinuous in the space variable. The presence of gravity also complicates the solution since the flux is no longer monotone and can also change sign. Here by using the idea of discontinuous flux in the space variable [1, 2], a numerical scheme is proposed and implemented. In the equation for s the dependence of the c_l variables is taken to lead to a discontinuous flux in the space variable. Then a Godunov flux called the DFLU flux can be written down for the discontinuous flux using previous ideas from [1, 2]. The discontinuity in permeability K and the effect of gravity is taken account of in a natural way and does not lead to any complications, with the DFLU flux retaining its very simple form in all cases, and hence being computationally very efficient. High order accurate scheme is constructed by introducing slope limiter in space variable and a strong stability preserving Runge-Kutta scheme in the time variable. The resulting schemes are shown to respect a maximum principle. Our numerical results are compared with other standard schemes on some canonical examples like the quarter 5-spot problem. The results from the exact Godunov flux for the system case is shown to be close to the results using the DFLU flux on some 1-D problems. The difficulties of handling the problem in a highly heterogeneous media in the presence of gravity attracts the importance of the proposed work.

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New Progress on Energy-Conserved S-FDTD Methods for Maxwell's Equations

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Maxwell's equations, which are a set of partial differential equations describing the relation of electric and magnetic fields, have been widely used in computational electromagnetics. They have been playing an important role in many applications such as the radio-frequency, microwave, antennas, aircraft radar, integrated optical circuits, wireless engineering, and the design of CPU in microelectronic, etc. During the propagation of electromagnetic wave in lossless media without sources, the electromagnetic energy keeps constant for all time, which explains the physical feature of conservation of electromagnetic energy in long term behavior. It is significantly important to preserve this invariance in time, for developing efficient numerical schemes for Maxwell's equations and specially for a long term computation of electromagnetic fields. In this talk, we will present our new progress on energy-conserved S-FDTD methods, including high-order energy-conserved schemes for Maxwell's equations and new energy-conserved schemes in metamaterials. We will talk theoretical results on energy conservation, stability and convergence and will give numerical examples to show their performance. Applications in metamaterials will also be introduced in the talk.

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B-Spline Collocation Software for PDEs with Efficient Interpolation-Based Spatial Error Estimation

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Over the past decade we have developed twomethod-of-lines B-Spline collocation software packages, BACOL and BACOLR, for the numerical solution of 1D parabolic PDEs. These packages have been shown to be efficient, reliable and robust, especially for problems with solutions exhibiting sharp layers, and for stringent tolerances. The packages feature adaptive control of estimates of the spatial and temporal errors. In BACOL the temporal integration and error control is handled by the BDF solver DASSL, while BACOLR employs the Runge-Kutta solver RADUA5.

While the BACOL/BACOLR spatial error estimates are generally quite reliable, the spatial error estimation algorithm involves the (expensive) computation of two collocation solutions of orders p and p+1. (The higher order solution is used to provide a spatial error estimate for the lower order solution.) This talk will discuss recent work investigating more efficient spatial error estimation algorithms based on (i) an order p+1 (superconvergent) interpolant that allows us to avoid the computation of the higher order collocation solution, and (ii) an order p interpolant (whose error agrees asymptotically with the error of the lower order collocation solution) that allows us to avoid the computation of the lower order collocation solution. We have implemented new, more efficient versions of BACOL and BACOLR based on these new error estimation schemes that we call BACOLI and BACOLRI. We provide numerical results comparing the original versions of BACOL and BACOLR with the new versions and show that the latter can be about twice as fast as the former.

Complex Dynamics of Population Behaviour (SS-CDPB)

Organizers:
Stephen Tully (University of Guelph)
Scott Greenhalgh (Yale University)
Chad Wells (Yale University)
Chris Pagnutti (University of Guelph)

Epidemiological & ecological modelling provides insight into the cost and effectiveness of control strategies; however, neglecting aspects such as behaviour can provide misleading information. The modelling of the complex interaction between behaviour and disease/ecological dynamics requires advanced mathematical techniques. The aim of this mini-symposium is to bring together modelling and computational approaches, including agent-based modeling, cellular automata, game theory, and hybrid dynamical systems, that demonstrate the impact of a population's behaviour on epidemiological, policy, ecology or economic outcomes.

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The evolution of competitive helping within biological markets

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Cooperation between unrelated individuals remains a puzzle in evolutionary biology. Recent mathematical and experimental work indicates that partner choice can select for high levels of helping (e.g. Barclay, 2011, 2013; Barclay & Willer, 2007). More generally, helping can be seen as but one strategy used to compete for partners within a broader biological market, yet giving within such markets has received little mathematical investigation. I will present game theoretical models whereby individuals help others to attract attention from them and thus receive a larger share of any help actively or passively provided by those others. The evolutionarily stable level of helping increases with the size of the biological market and the degree of partner choice. Furthermore, if individuals passively produce some no-cost help to partners, competitive helping can then invade populations of non-helpers because helpers directly benefit from increasing their access to potential partners. This framework of competitive helping demonstrates how high helping can be achieved, and why different individuals and different populations differ in their helpfulness.

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Equation-based and Agent-based models of adoption behaviour in multi-dimensional characteristic spaces.

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Modelling human decision processes and their impact on everyday life is today at the forefront of applied and social sciences. The process of decision making at the individual level has been studied extensively in operations research and management sciences, optimization, game theory, etc. The main traditional approach is concerned primarily with the study of appropriately defined static (equilibrium) states and their properties, assuming that individuals make rational decisions. For constantly evolving systems however, this is an important, yet not all sufficient, approach to describe aggregate behavior. This is a particularly important question if one studies adoption problems (such as new products, or new services or policy) in relation with a population's structure. In such a setting, the factors influencing individual and/or population attitudes are evolving, so the static theory cannot apply.

This talk is centred around two side-by-side dynamic modelling approaches to population behavior with respect to adopting green behaviour/policies (such as car share services or electronic waste recycling). In brief, we present time-dependent, multi-dimensional characteristic extensions of a standard static economic model of consumer choice for differentiated products reinterpreted for behaviour adoption. We use both an agent-based and a partial differential equations approach in order to incorporate social networks effects. In this setting, an individual's choice depends not only on its own attributes, but also on the choices of others in its social network, as well as their peers' influence in their personal decision making. Of central interest is how individuals react to the introduction of a new green service/policy what can be said about the specific adoption process of this such a new measure.

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The effects of vaccination preferences and perceived risk on the spread of influenza

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The simple ODE approach for modeling epidemics in a population often assumes a homogeneous populace that exhibits identical behavioural characteristics. However, the complexity of human vaccination behaviour can have a profound impact on the evolution of an epidemic as people (sometimes dramatically) change their stance towards vaccinate in accordance with a perceived morbidity of infection/vaccination[1]. Coupling vaccination behaviour and infectious disease dynamics is generally beyond the scope of compartmental ODE models. Fortunately, there exists a more general framework that allows for such an amalgamation of processes: hybrid systems.

We cast a compartmental epidemic model pertaining to the spread of seasonal influenza into the realm of hybrid systems. Through the use of hybrid systems and the concept of evolving group vaccination preferences, we attribute a physical process that describes the co-evolution of vaccination behaviour coupled with disease dynamics. The behaviour of vaccination candidates at a given event-time [3], is determined by shared perceptions of vaccination risk and a shared subgroup sensitivity to the current level of infection throughout the entire population. We examine the effects that different sensitivities have on the overall vaccine uptake with majority and minority group proportions and, in addition, demonstrate the potential impact vaccination behaviour may have on the stability of the hybrid system through Lyapunov stability theory [2].

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Ecological and Epidemiological Drivers of Viral Evolution

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While it has long-been recognized that disease transmission is impacted by human behavior, the consequences of human behavior on the ecology of directly transmitted pathogens has been understudied. Using a biophysical model of virus stability, we examine how much of virus evolution is driven by epidemiological factors, such as contact rates and protective behavior, and how much is driven by biological characteristics of the virus, such as its growth rate. We use agent-based models, which scale from local to planetary to elucidate the driving factors for both endemic and epidemic directly transmitted viruses.

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Outcome inelasticity and outcome variability in behavior-incidence models: an example from an SEIR infection on a dynamic network

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Behavior-incidence models have been used to model phenomena such as free-riding vaccinating behavior, where nonvaccinators free-ride on herd immunity generated by vaccinators. Here, we develop and analyze a simulation model of voluntary ring vaccination on an evolving social contact network. Individuals make vaccination decisions by examining their expected payoffs, which are influenced by the infection status of their neighbors. We find that stochasticity can make outcomes extremely variable and thus unpredictable: some stochastic realizations result in rapid control through ring vaccination while others result in widespread transmission. We also identify and explore the phenomenon of outcome inelasticity, wherein behavioral responses result in certain outcome measures remaining relatively unchanged. Finally, we explore examples where ineffective or risky vaccines are more widely adopted than safe, effective vaccines. This occurs when such a vaccine is unattractive to a sufficient number of contacts of an index case to cause failure of ring vaccination. As a result, the infection percolates through the entire network, causing the final epidemic size and vaccine coverage to be higher than would occur with a better vaccine. Effects such as extreme outcome variability and outcome inelasticity have implications for vaccination policies that depend on individual choice for their success and predictability.

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Modelling homophilic imitation with replicator equations

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Many social norms, which include behaviours, dress, and other cultural aspects of these traits, have no discernable benefit; they do not ostensibly increase the payoffs of the individuals. However, they may be greenbeards. Such tag-based effects have been used to explore the questions of how cooperation emerged amongst selfish individuals [1, 3], and how social groups are formed and evolve over time [2].

Here we develop homophilic replicator equations to model imitation dynamics with homophily. We assume that individuals have traits and strategies, where the strategies alone impact their fitnesses. We further assume that the population is non-structured and that individuals interact with one another to received payoffs that will determine their fitnesses. Inidividuals imitate others by comparing fitnesses, and imitating based upon these differences and the population densities. We factor in a component to model homophily, where individuals are more prone to imitate those who have similar traits. We set up an imitation replicator model to model these interactions and the changes in the group frequencies, dubbing this our homophilic replicator equation:

$$\dot{p}_i = p_i \left(\sum_{j=1}^{n} p_j((f_i - f_j)d_{ij} \right) \tag{1}$$

Where f_i and p_i are the fitness and density of population i. d_{ij} is the similarity of populations i and j in trait space.

We show the existence and characteristics of resulting fixed manifolds and conditions for stability. We discuss coat tailing, where trait densities at equilibrium are highly dependent upon the initial distribution of traits and strategies, and further implications for group formation. We extend our model to incorporate mutations/invasions and analyze a discrete version of the model.

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Parental decision-making towards childhood immunization and social norms

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It has been suggested that voluntary vaccination programs suffer from the free-riding problem ensued from the public perception of herd immunity, which leads to a decrease in the vaccination acceptance rates and epidemic reemergence. Association between vaccines and severe side effects, true or false, results also in a decline in vaccine uptakes. Pertussis vaccination campaign in the UK, for example, suffered from a precipitous fall due to its questionable linkage to neurological diseases in the early 70s. The current pertussis vaccine uptake in the UK, however, exceeds the WHO's recommended target of 95%. In this research we developed coupled disease and behavioral models to describe incidence of childhood diseases and immunization acceptance in the process of parental decision-making. Those decisions are based on the personal variables: perceived vaccine risk and efficacy, and perceived risk of infection. According to the Health Belief Model, parents make their decision based on social variables, namely social norms and group pressure, in addition to those personal variables. In my talk, I will present an extension to the coupled behavioral-disease model to include the social norms and group pressure. I will also present stability analysis and simulation results of the model, showing how the model can more convincingly explain the range of observed dynamics than certain previous models.

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Outlook on a global forest transition

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The decline of the Earth's forest cover and other natural habitats has been a subject of great concern in recent decades. According to the Food and Agriculture Organization of the United Nations (FAO), the global forest cover was reduced by more than 70 MHa since 1990, an area larger than France and roughly 0.5% of the global land area. The main driver of deforestation is agricultural expansion. Despite the apparent demise of the world's forests, over the last two centuries many countries, particularly in the industrialized world, have experienced a forest transition (FT); that is, a transition from a period of shrinking forest area to a growing one. Most studies of the FT and forest decline focus on spatial scales at the national and sub-national levels, and on temporal scales of a few decades, but there are some important notable exceptions. In particular, these studies have focused on policies and drivers that could potentially either trigger or inhibit a global forest transition in the future, but few quantitative claims have been made pertaining to the timing of the forest transition and to the ultimate scale of deforestation. Here, we develop a mathematical model to address these issues.

We show that the world food equation accounts for almost all of the land use changes that have occured during the past millenium. Our model fits surprisingly well historic data on forest cover, human population and agricultural yield dynamics. We extrapolate on these findings to postulate conditions under which a global forest transition may occur. We find that under most circumstances a forest transition is not likely to occur without radical new advancements in agricultural technology. However, if agricultural yields and per capita consumption continue to increase as they have in the last half-century, then a forest transition may occur within the next century, depending on the level to which per-capita food consumption increases during the same period. We discuss that reducing food wastage and consumption is just as effective for land sparing as is increasing yields.

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Agent-Based Modeling of Emotional Communications in Online Social Networks: The Role of Offline Processes in Online Bursting Events

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Online communications are now days utilized by a large fraction of the world population for exchange of ideas, information and emotion, frequently leading to an intricate dependency between offline and online behaviors of users. The prominent examples are the online social networks with their predefined "social" structure, which constraints potential exchange of messages. Huge amount of digital data of high resolution exits about users' online activity. The data on social network dialogs have been researched as a complex system in the physics laboratory [1]. Quantitative analysis of the data, by statistical physics combined with machine learning methods of text analysis, revealed the occurrence of temporal correlations significant for the collective behaviors of users in which emotion carried in the text of messages plays an important role [1].

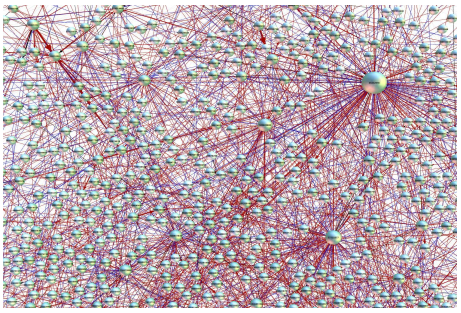

Figure 1: A part of social network `MySpace` with users, shown as nodes, exchanging emotional messages along the "friendship" links.

In this paper, we study the underlying mechanisms in the dynamics by means of agent-based modeling [2]. Our focus is on the occurrence of bursting events of emotional messages and the effects of external processes on them. In the first part, we provide details of key difficulties in this modeling approach. We briefly present the implementation of the model, in which several features of agents are inferred from the empirical data. In the model, the agent's emotional state variables [2] evolve under aggregated influence fields of the received messages along their connections in the network. The simulations are performed at a very large empirical network constructed from the data of dialogs in `MySpace` (Fig. 1). Varying the type and strength of noise in the dynamics, we determine the distributions of size and duration of avalanches (bursts) comprising the emotional messages. Furthermore, we identify the parameters which control their appearance and determine statistical properties of the triggering fields.

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Chaos in an unforced Malaria Model

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Chaotic dynamics have rarely been reported in deterministic continuous time mathematical models for malaria, unless when seasonal forcing is included in the model. We showed that when focus is placed on the mosquito vector in the malaria transmission process so that the mosquito feeding pattern, demography and reproduction habits are explicitly incorporated in the transmission dynamics, an unforced deterministic malaria model exhibited complex dynamics (see Refs. [1, 2]). In particular, when the reproductive gains that accrue to the mosquito's population as a result of its interaction with the human population is accounted for, a non-seasonally forced mass action continuous time deterministic malaria model was shown to be oscillatory and it exhibited the phenomenon of backward bifurcation (see Refs. [1, 2]). When a more nonlinear birthrate function for the mosquito population was considered, chaotic dynamics were observed. We posit that mathematical models for malaria and other vector-borne diseases should be modeled to account for the reproductive gains to the vector's population as a result of its interaction with the human or host population.

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Coevolution of risk perception, sexual behaviour, and HIV transmission in an agent-based model

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Risk perception shapes individual behaviour, and is in turn shaped by the consequences of that behaviour. Here we explore this dynamic in the context of human immunodeficiency virus (HIV) spread. We construct a simplified agent-based model based on a partner selection game, where individuals are paired with others in the population, and through a decision tree, agree on unprotected sex, protected sex, or no sex. An individual's choice is conditioned on their HIV status, their perceived population-level HIV prevalence, and the preferences expressed by the individual with whom they are paired. HIV is transmitted during unprotected sex with a certain probability. As expected, in model simulations, the perceived population-level HIV prevalence climbs along with actual HIV prevalence. During this time, HIV- negative individuals increasingly switch from unprotected sex to protected sex, HIV+ individuals continue practicing unprotected sex whenever possible, and unprotected sex between HIV+ and HIV- individuals eventually becomes rare. We also find that the perceived population-level HIV prevalence diverges according to HIV status: HIV- individuals develop a higher perceived HIV prevalence than HIV+ individuals, although this result is sensitive to how much information is derived from global versus local sources. This research illustrates a potential mechanism by which distinct groups, as defined by their sexual behaviour, HIV status, and risk perceptions, can emerge through co-evolution of HIV transmission and risk perception dynamics.

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Policy resistance undermines superspreader vaccination strategies for influenza

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Highly connected individuals (superspreaders) have been found to be a major influence on the spread of disease; this small sub-population is responsible for the majority of the infections that occur in an epidemic. Theoretical network models have found vaccinating superspreaders to be a highly effective and efficient way to reduce incidence. One issue with these models is the assumption that a superspreader is always willing to vaccinate; not allowing a model to capture the feedback that occurs between incidence and vaccination behaviour can allow the new policy to seem more beneficial than it truly is. This can be problematic for diseases like influenza, where vaccination is voluntary and vaccine coverage is below the desired level.

We have coupled disease and vaccination behaviour dynamics for influenza on an empirically based network under numerous vaccination strategies, most of which are designed to target superspreaders. We have taken a psychologically structured approach towards vaccination behaviour for influenza. An individual's decision to vaccinate is influenced by their perceived past infections, vaccine complications and vaccine efficacy; the individual's perceptions and decision to vaccinate can be swayed by the perceptions of others in the population. Our objectives are to understand: 1) whether the vaccination strategies targeting superspreaders are still effective when behaviour is accounted for; 2) whether economic incentives improve the effectiveness of these strategies; and 3) how perceived vaccine efficacy and decisions are determined by the vaccine-disease dynamics.

We found behavioural feedbacks reduce the effectiveness of superpsreader strategies; by targeting superspreaders the incidence of influenza is reduced, making vaccination less appealing to others (non-superspreader) next season. Introducing an economic incentive into the vaccination policies did improve their effectiveness slightly; however, any benefit from the incentives was lessened by policy resistance and the savings from the reduction of incidence was outweighed by the cost of incentives.

Our results suggest special care should be taken in designing influenza vaccine policies targeting superspreaders, with or without economic incentives, due to policy resistance caused by behavioural feedback.

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Modelling Awareness and Adoption: Aggregate Behaviour versus Agent-Based Interactions with Network Effects

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We construct and examine a model of adoption of a product or policy using, firstly, a system of differential equations and then secondly, through simulation, an agent-based model. Awareness must come before adoption, and we model this as a simple epidemic type model, where information is spread through advertising and contact with other agents in the population. Adoption is then conditional on awareness and occurs only if the agent finds the perceived cost acceptable. After simulating the system using an agent-based model, we introduce heterogeneity through the model parameters, which are then considered individual attributes and include influence rates, effectiveness of advertising, price sensitivity, and speed of adoption.

In the DE model, it became clear that the advertising effect, c, had the most effect on the length of time it took for the model to reach its equilibrium. Influence rates, b and b", and the speed of adoption rate, k, had a small effect on how fast awareness and adoption took place within the first 100 time steps. The price sensitivity, d, was the only parameter to affect the resulting equilibrium point. As expected, a high price sensitivity and thus high perceived price meant that very few individuals adopted overall and awareness took longer to completely diffuse; whereas a low price resulted in individuals becoming aware very quickly and the population consisting of almost only adopters in the end.

We also examine the effects of various network topologies by organizing individuals into lattice and preferential attachment networks. We first found that as we increased the population size, our model regressed to the mean and resulted in an outcome very close to that of the DE model. Individualizing each parameter resulted in adoption that was very similar to the patterns of adoption in the DE model. We noted that it resulted in slower awareness over time, with advertising effect once again having the greatest consequence. Individualizing the price sensitivity influenced the equilibrium point slightly, resulting in a slightly higher amount of adoption. Adding different network types, specifically lattice and preferential attachment networks, did little to influence adoption over time. They did, however, have a slight effect on slowing down the diffusion of awareness.

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Adaptation and the evolution of parasite virulence in an increasingly connected world

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Today, humans can travel on spatial scales never before seen in their evolutionary history. In turn, this tremendous ability to travel has meant that infectious diseases of humans can now be readily transmitted over great distances. While the public health challenges of disease transmission on large geographic scales is well appreciated, the long-term consequences for the evolution of microparasitic infections of humans is not. In this talk I will outline a simple model for the evolution of microparasite virulence in a geographically structured population of hosts, e.g. humans [1]. The model itself can be treated as a branching process [2], and the analysis relies heavily on W. D. Hamilton's notion of *inclusive fitness* [3]. I find that, as geographic structure is eroded, selection favours increased parasite virulence. In addition to its obvious public health implications, the result sheds light on general rules of adaptation in nature.

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Incentives' Effect in Influenza Vaccination Policy

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Influenza, the most common upper respiratory illness, leading to an annual infection rate of 5-15% in developed countries [1]. In the U.S. alone, the disease is responsible for taking overall 610,660 years of life, 3.1 million hospitalized days, and 31.4 million outpatient visits each year [2]. Vaccination is considered the most promising public health measure for reducing the burden of the disease. In the majority of developed countries, the level of influenza vaccination coverage in all age groups is sub-optimal. Hence, the authorities offer different kinds of incentives for people to become vaccinated such as subsidizing immunization or placing immunization centers in malls to make the process more accessible.

We built a theoretical epidemiological game model to find the optimal incentive for vaccination and the corresponding expected level of vaccination coverage. The model was supported by survey data from questionnaires about people's perceptions about inuenza and the vaccination against it. Results suggest that the optimal magnitude of the incentives should be greater when less contagious seasonal strains of influenza are involved, greater for the non-elderly population rather than the elderly, and should rise as high as $57 per vaccinated individual so that all children between the ages of six months and four years will be vaccinated.

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Computational Fluid Dynamics for Real Applications (SS-CFDRA)

Organizers:
Lakhdar Remaki (BCAM)
Stéphane Moreau (Université de Sherbrooke)
Abdelkader Baggag (Université Laval)

CFD (Computation Fluid Dynamic) analysis has made significant inroads in industrial applications thanks to the important increase of computer capabilities along with the improvement of the underlying numerical methods and visualization tools. The CFD discipline is essentially based on the numerical discretization of the Navier-Stokes equations that describe the fluid motion. Even if these equations are known since more than 150 years and despite the availability of powerful computing supercenters, a simulation of a complex fluid dynamic still a challenging task, especially for phenomena that occur at very small scales like turbulence, vortices and aero-acoustic structures. The CFD special session will cover any work related to fluid dynamic including any advances in numerical analysis aspects, modeling, related fields like aero-acoustics, aero- elastics, gas-particles interactions and any coupling with Navier-Stokes equations. Works showing the application to complex geometries and the role and trend of CFD in industry are encouraged.

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A robust computational procedure for nonlinear thermo-electrical problems in fractured media based on XFEM

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Thermo-electrical effects in fractured media are encountered in many situations of practical interest; and the numerical treatment of this physical phenomenon has run into difficulties due to the temperature and voltage discontinuity.

In this presentation, a general computational procedure, which is based on the eXtended finite element method (XFEM), is proposed to efficiently deal with transient and nonlinear problems, and to estimate field distributions in cracked medium.

The finite element approximation is enriched in order to take into account the crack discontinuities due to the jump and the asymptotic near-tip function, using the partition of unity method. And the discretization results in a nonlinear system that is solved using the Newton-Raphson algorithm.

Different numerical examples show the high accuracy and the robustness of the proposed computational procedure in efficiently capturing the temperature and voltage jumps across the crack.

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Magnetic field effect on the natural convection flow in a cavity

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The steady, two-dimensional and laminar magnetohydrodynamic (MHD) natural convection flow in the presence of radiation and viscous dissipation is considered in a square cavity filled with a porous medium. The flow prediction inside the porous medium follows Darcy's model and is subjected to an inclined uniform magnetic field. The vertical walls of the enclosure are kept at constant temperatures while the top and bottom walls are considered thermally insulated. The properties of the fluid and porous medium are homogeneous, isotropic and constant except variation of fluid density with temperature. The fluid and porous medium are in thermal equilibrium and radiative heat flux in y direction is negligible in comparison to that in the x direction. The non-dimensional form of the governing equations are given as:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2} = -Ra\frac{\partial\theta}{\partial x}-Ha^2\left[\frac{\partial^2\psi}{\partial y^2}\sin\varphi+2\frac{\partial^2\psi}{\partial x\partial y}\sin\varphi\cos\varphi+\frac{\partial^2\psi}{\partial x^2}\cos^2\varphi\right]$$

$$\frac{\partial\psi}{\partial y}\frac{\partial\theta}{\partial x}-\frac{\partial\psi}{\partial x}\frac{\partial\theta}{\partial y} = (1+\frac{4R}{3})\frac{\partial^2\theta}{\partial x^2}+\frac{\partial^2\theta}{\partial y^2}+\varepsilon\left[(\frac{\partial\psi}{\partial y})^2+(\frac{\partial\psi}{\partial x})^2\right]$$

where φ is the angle between the magnetic field and x-axis, ψ and θ are the stream function and the temperature, Ra and Ha are the Rayleigh and Hartmann numbers, ε and R are the viscous dissipation and radiation parameters, respectively.

The dual reciprocity boundary element method (DRBEM), which is a boundary only discretization technique, is applied for the solution of the non-dimensional governing equations with appropriate boundary conditions for the flow and the temperature. Constant elements are used for the discretization of the boundary of the cavity. Numerical calculations are carried out for wide ranges of Hartmann and Rayleigh numbers at various magnetic field orientation angles. The numerical results are presented for different values of governing parameters, namely, viscous dissipation and radiation to analyze the effects of them on the flow behavior and the temperature. The flow is significantly affected especially at the core of the cavity and the flow field circulation decelarates with an increase in Hartmann number. Moreover, the core of vortices is converted from the vertical position to the horizontal position as the angle of the external magnetic field increases from zero to $\pi/2$, whereas there is no significant effect of the magnetic field orientation on the isotherms. It is also observed that an increase in radiation results in an incrase in the average Nusselt numbers at both hot and cold walls. On the other hand, average Nusselt number decreases on the hot wall following an increase in the viscous dissipation parameter while it develops it on the cold wall. These results are in good agreement with the other published results.

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Design Considerations for Thermal Management of Electronics Enclosures

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This study focuses on the design and optimization of an electronics enclosure intended for operation in an outdoor commercial heating, ventilation and air conditioning, HVAC, application. In particular the designed was optimized for a high ambient environment without the aid of forced air cooling. As electronically controlled motor drive systems are increasing in use, designs need to operate in new challenging environments, reach higher power density, and enable higher levels of system integration. Computational Fluid Dynamics, CFD, was used for design, analysis and optimization and correlated with test data. A design of experiments, DOE, was used to evaluate the sensitivity of the final design to the operating environment. A constrained optimization was performed to determine the optimal fin spacing, height, angle and thickness of the enclosure geometry for thermal dissipation of the heat from the power electronics. Various fin topologies were also analyzed to evaluate the impact of increased surfaced area and enhanced thermal mixing effects. After a thorough review of the design space, general design recommendations are made and an optimized design reviewed.

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A CFD Optimization of Airflow Efficiency for an Electric Motor Driven Centrifugal Fan System for Residential HVAC Applications

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This study focuses on the design and optimization of an electronics enclosure intended for use in a centrifugal fan being driven by an electric motor for the residential HVAC market. Typically in these systems, the motor is mounted directly in the airstream of the centrifugal fan, but in this case the Regal Beloit's axial motor technology allows for the minimization of this obstruction to the airflow. In the system analyzed the axial motor is mounted in the center of the centrifugal fan and the electronics used to drive the system is enclosed and mounted to the axial motor. This enclosure has been optimized for system airflow efficiency and thermal management of the electronics. A sensitivity analysis was also performed to understand the optimized design's performance under various application environments. Computational fluid dynamics, CFD, was used as a test platform and tool for optimization. The CFD analysis was driven by goal optimization software to explore the design space and lead to an optimized design for overall efficiency. Results were validated to test data and test visualization methods. This presentation will cover the design requirements and details of the application, the optimization and CFD techniques used and the criteria used for CFD model validation.

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Non-equilibrium solidification in undercooled faceted-faceted Ni-56.2 Si at % eutectic alloy

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The maximum undercooling of 316 K was achieved in the bulk liquid Ni-56.2 at% Si eutectic alloy (faceted-faceted NiSi-NiSi2 eutectic alloys) melts through glass fluxing combined with cyclic superheating, in which a typical transition of faceted-faceted (FF) NiSi-NiSi2 eutectic takes place. A wide variety of microstructures can be obtained in the FF NiSi-NiSi2 eutectic alloys with the increase of undercooling. The metastable Si phase was obtained through slow post-solidification when undercooling $\geq$ 14 K, and it is confirmed by optical microscope (OM), scanning electron microscope (SEM) with an electron probe microanalysis (EPMA) and differential scanning calorimetry (DSC).

Based on the principle of minimum free energy and transient nucleation theory, the phase selection of melt was discussed with regard to the metastable phases formation in the bulk undercooled FF NiSi-NiSi2 eutectic alloys. In this paper, the formation of metastable phases from undercooled FF NiSi-NiSi2 eutectic alloys was determined by the competitive nucleation with undercooling, i.e., high undercooling facilitates the preferential nucleation of metastable phases.

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Modeling of Bubble Motion in a Sound Field

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We study the interaction of the motion of an expanding and translating bubble with a sound field, using the method of effective potential adopted by Landau and Lifshitz. Rayleigh [1] studied the adiabatic expansion of a spherical gas bubble in an inviscid fluid. He derived the differential equation for the growth of the radius R(t) of the bubble. Plesset [2] modified this equation to include the viscosity of the outside liquid. The motion of a gas bubble, which translates with velocity U as it expands, has been considered by Chakraborty [3] and Chakraborty and Tuteja [4], assuming a spherical bubble shape. Detailed numerical results have been given in Ref. [4] when the pressure in the liquid far from the bubble is constant. In the absence of the translational motion of the expanding bubble, its motion in a sound field has been discussed by Lauterborn [5] and Keller and Miksis [6]. In the present paper, we investigate the interaction of the motion of an expanding and translating bubble with a sound field. In our study we shall use a method applied by Landau and Lifshitz [7] in their study of stability of an inverted pendulum when the pivot oscillates vertically. This method has been discussed by Blackburn, Smith and GrØnbeck-Jensen [8]. In this method the concept of an "effective potential" is used. The oscillating amplitude of the pivot is taken as small and the period of oscillations is assumed to be small compared to a characteristic period of the pendulum. Using the same method, in our discussion of the bubble motion in a sound field, we work under the assumption that the amplitude of the sound field is small, while the frequency of this field is large compared to a characteristic frequency of the oscillation of the bubble. We find that the equilibrium value for the mean radius R of the bubble exhibits a bifurcation [9] as the sound field amplitude increases from a critical value which is zero or nearly so.

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CFD Simulation of Biomass Gasification using Circulating Fluidized Bed by Eulerian-Eulerian Approach

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In this work, a 3-D steady CFD (computational fluid dynamics) model via the Eulerian-Eulerian approach is established to simulate the process of biomass gasification using a circulating fluidized bed. The simulation results, including the temperature and concentration profiles, are analyzed and compared with the literature data. A grid analysis is conducted to investigate the grid independence for the CFD model by comparing the simulation results from different highresolution grids. Three types of turbulence models, standard, RNG, and realizable k-epsilon equations are applied to investigate the impacts of turbulence on the simulation of gasification process. The influences of radiation are also studied by comparing the gasification models with and without radiation mode. Various equivalence ratios are analyzed to study the reaction kinetics of gasification and achieve the optimal settings for the process.

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Dendritic Growth Velocity Calculation and Microstructural Evolution of Ni-Cu-Si Alloy

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Ni-based alloys have been extensively utilized in the fields of aerospace and marine manufacture [1] due to their excellent performances. Dendrites are usually formed during preparing this kind of alloys [2]. The dendritic growth is fundamentally required to understand microstructure evolution and to explore its effect on the mechanical properties. However, it is extremely difficult to obtain the data of growth velocity by undercooling experiments [3]. The aim of this work is to investigate the microstructure evolution and the dendritic growth velocity dependent on undercooling, in which ternary $Ni_{80}Cu_{10}Si_{10}$ alloy is selected. LKT/BCT model [4] is employed to compute the growth velocity, and corresponding solidification experiments are also performed.

The dendritic growth velocities of $Ni_{90}Cu_{10}$ and $Ni_{90}Si_{10}$ alloys are derived by using LKT/BCT model, as shown in Figure 1. It can be observed that the growth velocity increases with the rise of the undercooling. Moreover, the growth velocity of $Ni_{90}Cu_{10}$ alloy is always larger than that of $Ni_{90}Si_{10}$ alloy. Figure 2 illustrates the solidified microstructure of $Ni_{80}Cu_{10}Si_{10}$ alloy.

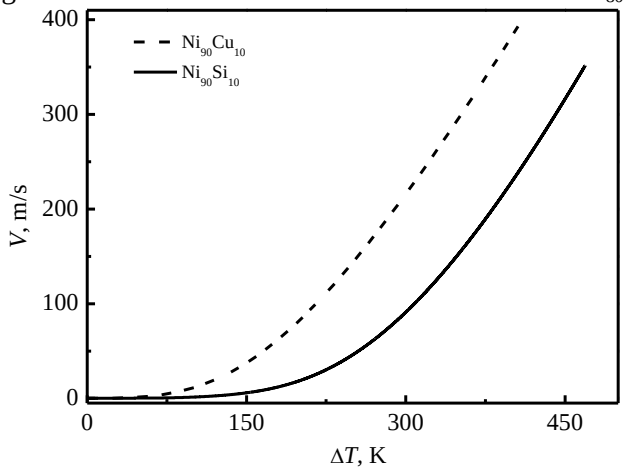

Figure 1: Calculated growth velocity of dendrite in $Ni_{90}Cu_{10}$ and $Ni_{90}Si_{10}$ alloys.

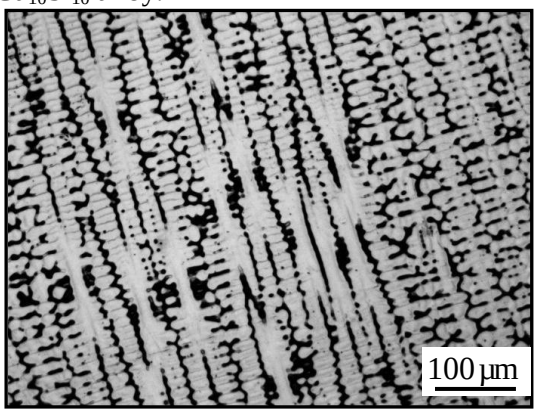

Figure 2: Solidified microstructure of $Ni_{80}Cu_{10}Si_{10}$ alloy.

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Wake Topology for Steady Flow past an Inclined Elliptic Cylinder

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The flow of an incompressible viscous fluid past an elliptic cylinder with minor-to-major axis ratio of 0.2 and at incidence to the free stream is considered. Previous solutions of this problem, e.g. Refs. [1,2], have been limited to Reynolds numbers Re up to 40. The objective of the present research has been to obtain solutions for higher Re to permit completion of a bifurcation diagram presented by Ref. [1], which describes the wake topology behind the cylinder in terms of three regions: Region I with no separation, Region II with a single attached recirculatory region, and Region III with two recirculatory regions, one attached and the second unattached to the cylinder.

The two-dimensional Navier Stokes equations in stream function/vorticity formulation are solved using a finite difference scheme employing two grids, one that covers the full flow domain and a second that maps onto the wake region behind the cylinder. Numerical solutions have been obtained using grid resolutions up to 160x320 for the radial/angular coordinates for Re up to 450. Solutions for the symmetric flow past a circular cylinder have also been obtained for Re up to 300 and compared with Ref. [3].

For the cylinder at 0^0 incidence, initial separation with formation of two separation bubbles is found to occur at approximately Re = 200, in close agreement with Ref. [4]. The lengths of the separation bubbles increase with Re increasing above 200. When a small angle of incidence is introduced for some Re just greater than 200, the flow transitions to Region III topology with a single attached separation bubble complemented by a second unattached recirculatory region. The size of these recirculatory regions is found to decrease with increasing incidence until the unattached recirculatory region disappears thereby giving a Region II topology The attached recirculatory region continues to decrease in size with further increases in incidence until it also disappears yielding Region I topology. Further increases in incidence then lead to the behaviour reported by Ref [1]. The range of incidence angle over which this behaviour is present decreases with increasing Re until, at Re above 230, the wake topology consists of Region III, Region II and Region III with increasing incidence angle, i.e. the flow is separated for all incidence angles.

The results obtained have permitted extension of the bifurcation diagram presented by Ref. [1] for Re up to 450 with completion of the region transition curves. The trend of the findings are in agreement with predictions by Ref. [2] of a non-monotonicity in the relationship between incidence angle and Re for initial separation, these being based on the linearity property of eddy length with Re. The non-monotonic solution behaviour for Re > 200 with incidence angle increasing from 0^0 is of interest, particularly in how the separated bubble initially decreases in size and disappears before reappearing again.

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[1] Currently attached to the NATO Communications and Information (NCI) Agency. The work reported here is a continuation of Ph.D. research conducted at the University of Western Ontario and does not reflect official work/views of the NCI Agency.

Control Methods for Advanced Industrial Systems (SS-CMAIS)

Organizers:
Behzad Samadi (Maplesoft)
Jurgen Gerhard (Maplesoft)

Advanced control systems have to meet progressively tighter standards on performance and safety. In addition, the manufacturers compete to increase the quality of their products and at the same time, reduce the cost of development and manufacturing. Model based product design methods decrease the need for extensive testing and calibration. They also decrease the time and cost of development and increase the reliability of the final product. The objective of this session is to stimulate productive discussions between mathematicians and engineers to find innovative solutions for real-world problems. Suggested topics include but are not limited to: polynomials in control theory, symbolic model simplification, piecewise affine systems, reachability analysis, hybrid systems, symbolic nonlinear control synthesis, parametric robust control, optimal control, distributed algorithms, formal verification, robotics, and advanced automotive control systems.

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Model Predictive Control via Triangular Decompositions of Semi-Algebraic Systems

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In many industrial and engineering applications, process control plays a central role. Among the possible control strategies, model predictive control (MPC), also called receding horizon control (RHC), stands out for its excellent ability to handle constraints. While MPC has been successfully applied to many industrial applications, further developments are limited when it becomes necessary to solve many large on-line optimization problems. To overcome this situation, parametric optimization is often used such that most of the computation burden is pushed to an off-line phase.

In this talk, we discuss two methods, based on symbolic computation, to perform parametric optimization, together with the corresponding on-line strategies, targeting MPC in the case of polynomial constraints and objective function. These methods rely on tools for solving systems polynomial equations and inequalities, taken from the theory of triangular decomposition. The first method is a general purpose tool relying on a new scheme for computing cylindrical algebraic decomposition. The second one, under some genericity assumptions, leads to attractive running time estimates.

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Symbolic Methods in Control Theory

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We will give an overview presentation of symbolic computation approaches that have been used for control analysis and design, in particular, robust control and synergetic control. The methods presented make use of symbolic computation techniques from linear algebra, as well as complex and real algebraic geometry, such as Gröbner bases and Cylindrical Algebraic Decomposition. A key construction employing the latter methods is to rephrase the control problem as a system of polynomial equations, inequations, and inequalities, where some of the variables are existentially or universally quantified.

The presentation will also include a discussion of the challenges of using symbolic methods, and a summary of current research at Maplesoft related to symbolic control.

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Discovering Lyapunov Functions for Dynamical Systems Using Simulation

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Model-based development (MBD) is a popular process for designing, implementing, and testing embedded software designs for real-time control systems and is used in many sectors, such as automotive. Verifying correctness of MBD designs is a difficult task and is essential for ensuring that the system satisfies safety constraints. Dynamical systems analysis techniques can be applied to MBD designs to verify system properties, such as stability or performance bounds, but these techniques are rarely used in any but the earliest stages of the MBD process [1, 2].

We present a technique that allows the designer to verify stability and to predict performance bounds for MBD designs and can be applied at several stages of the MBD process [3]. The technique leverages Lyapunov analysis, semidefinite programming, and global optimization to automatically discover correctness certificates. Our technique is more practical than traditional techniques based on Lyapunov analysis, in that it can be applied directly to system models (e.g., Simulink® models) without requiring an analytic representation of the system dynamics.

Our technique is based on the following observation regarding a dynamical system given by $\mathbf{x}_{k+1} = f(\mathbf{x}_k)$. Given a collection of pairs of points $(\mathbf{x}_i, \hat{\mathbf{x}}_i)$, where $\hat{\mathbf{x}}_i = f(\mathbf{x}_i)$ for each i, a necessary condition for Lyapunov stability is the existence of a function $v(\cdot)$ that satisfies the following over some domain D:

$$v(\mathbf{x}) > 0 \qquad \forall \mathbf{x} \neq \mathbf{0},\ v(\mathbf{0}) = 0, \tag{1}$$

$$v(\mathbf{x}_i) - v(\hat{\mathbf{x}}_i) > 0 \qquad \forall i. \tag{2}$$

The technique can be summarized as follows. Simulation traces are used to construct a Lyapunov function candidate ($v(\cdot)$), where the candidate functions are restricted to the class of Sum of Squares (SoS) polynomials [4], and semidefiniete programming is used to ensure (1) and (2) are satisfied. Next, a global optimizer is employed to provide a refutation of the Lyapunov candidate. If a refutation is found, then the refuting simulation trace is added to the collection of simulation traces and an updated Lyapunov candidate is computed. This process continues until either a.) no refuting simulation trace is found or b.) a computation budget has been reached.

In this talk, we describe the above procedure and present an implementation that is applied directly to Simulink models. We present several examples showing that we can automatically discover Lyapunov functions for Simulink models of nonlinear systems. We conclude with a discussion of open questions and direction for future work.

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Using Kernel Module Bases for Fast Polynomial Matrix Arithmetic

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Polynomial matrices appear in control theory as transfer function matrices of linear dynamical systems. In this talk we show how bases of kernels of matrix polynomials, considered as modules over the entries of the matrices can be used for fast, deterministic algorithms for polynomial arithmetic. In particular we show how kernel bases can be used for computation of inverses, column bases and matrix normal forms. Combining this with the fast kernel basis algorithm of Zhou-Labahn-Storjohann gives optimal algorithms for the previously mentioned computations.

This is joint work with Wei Zhou.

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Transverse feedback linearization and exterior differential systems

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Many control objectives can be accomplished by stabilizing an appropriate invariant set in the state space of a control system. This point of view is relevant in applications such as output regulation [1], synchronization [2], formation control problems for multi-agent systems [3] and path following. A natural approach to stabilizing sets is to seek a smooth function that yields a well-defined relative degree and whose associated zero dynamics manifold coincides with the set to be stabilized. If such a function exists, then, using input-output feedback linearization, the set stabilization problem reduces to the problem of stabilizing the origin of a linear time-invariant system. This process is called transverse feedback linearization and the function is called a transverse output function.

Consider an invariant, smooth, embedded submanifold Γ in the state space of a smooth, nonlinear, autonomous, deterministic, finite-dimensional, single-input control-affine system

$$\dot{x} = f(x) + g(x)u, \qquad f,g : \mathbb{R}^n \to \mathbb{R}^n \text{ smooth }, \qquad u \in \mathbb{R} \text{ the control input.} \tag{1}$$

The results in [4] provide necessary and sufficient conditions for the existence of a function $\lambda : \mathbb{R}^n \to \mathbb{R}$ with the properties discussed above. Namely, λ yields a well-defined relative degree for system (1) on the target set Γ and the associated zero dynamics of (1) with output λ, equals Γ. While the conditions in [4] can be checked to guarantee the existence of the function λ, the process by which the function is computed is not constructive. In other words, even if the function is guaranteed to exists, it may be very difficult to find.

In the present work, we aim to leverage ideas from the field of exterior differential systems, in particular the work of Gardner and Shadwick [5], see also [6], to generate dual conditions for the existence of a transverse output function. The motivation for this is twofold. First, the dual conditions of [4] may provide further geometric insight into the problem. Second, by adapting the symbolic algebra algorithm in [5] to the present problem, it is hoped that the process of finding the transverse output function is simplified.

The above research program is in its infancy and as such this talk focuses on the formulation of the problem. We motivate the research, discuss the relationship between feedback linearization and exterior differential systems, review the Gardner-Shadwick algorithm, and present research directions for its application to transverse feedback linearization.

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An optimal predictive control strategy for a plug-in hybrid electric powertrain

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Plug-in hybrid electric vehicle (PHEV) development seems to be essential for a sustainable transportation system along with electric vehicles. An appropriate power management strategy for a PHEV determines how to blend the engine and the battery power in such a way that leads to significant fuel economy improvement and environmental footprint reduction. Among the proposed strategies in the literature, the model predictive control (MPC) approach suggests a suboptimal solution to this problem and is able to handle hard constraints on control and states. The only serious drawback of this method is the expense of calculations for any time step of control and consequently limitations for implementing this approach on a commercial control hardware with a limited amount of CPU power and memory size. For resolving this issue, the explicit model predictive control (eMPC) approach has been proposed in the litrature. In the eMPC approach, the optimal control problem is solved offline and the results are stored as look up tables. This will significantly reduce the controls calculation time during plant operation. In this research, we use the eMPC approach to design an optimal and real-time implemetable power management strategy for a PHEV powertrain. By using an appropriate control-oriented model we can formulate the eMPC problem [1] to minimize the fuel consumption (see Eqs. (1)) while maintaining drivability and tracking a predefined battery state of charge trajectory.

$$min_U \left\{ \sum_{j=1}^{N_p} \left[X^T(j) Q X(j) + U^T(j) R U(j) \right] \right\} \tag{1}$$

In the above cost function, N_p is the length of prediction horizon, Q and R are the weighting parameters. X is the state vector, and U is the control vector consisting of the battery, the engine and braking power.Based on the optimum-operating line (OOL) of the engine we can find appropriate controls and apply them to the plug-in hybrid electric powertrain model, which results in the following figure. As seen in Fig. 1, the battery state of charge drops to the minimum possible level at the end of the trip. Therefore, the controller has maintained drivability and also kept the final SOC above the minimum level and the simulation time is faster than real-time.

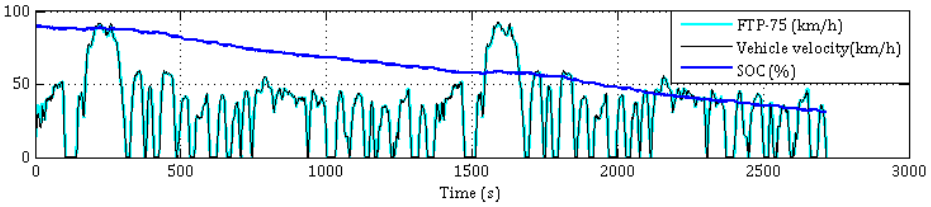

Figure 1: Vehicle velocity and battery state of the charge (SOC) trajectory along two successive FTP-75 drive cycle.

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Computational Materials Science (SS-CMS)

Organizers:
Haipeng Wang (NPU and University of Toronto)
Ziad Saghir (Ryerson University)

The in-depth application of computational science has led to many significant results in the field of materials science. A variety of computational methods, such as First Principle, Molecular Dynamics, Monte Carlo, and Phase Field, to name just a few, have been widely employed to investigate microstructure evaluation, heat and mass transfer processes, catalytic conversion and relationship between micro or nanostructure and property, etc. Computational science is playing an important role in observing and predicting crystal growth, phase transition, thermodiffusion, thermal expansion, mechanical properties, atomic structure, metallic glass formation and band gap, etc. It has become a powerful approach to develop novel materials. Many problems in diverse areas of computational materials science require dealing with multiphysics/multifield models, while modelling approaches are frequently based on multiscale techniques. This special session of computational materials science aims to share the updated achievements and to discuss the future development of applying computational science in materials science, which will relate to various metallic alloys, inorganic and organic materials.

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Nucleation Heterogeneity in Shape Memory Alloys: Studies with 3D Coupled Thermo-Mechanical Phase-Field Models

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The microscopic defects, such as heterogeneous nucleation, play an important role in phase transformation characteristics of shape memory alloys (SMAs) [1, 2]. In this contribution, we present studies of the effect of heterogeneous nucleation on the martensitic phase transformation in SMAs by using a 3D coupled thermo-mechanical model. The model is developed based on the phase phase-field theory and the Ginzburg-Landau free energy to describe the cubic-to-tetragonal phase transformations in SMAs. It has a bi-directional coupling in the thermal and mechanical physics via strain, strain rate and temperature. The nonlinear hysteresis has been described via higher-order polynomial terms and phase transformations using fourth-order differential terms [3]. A variational form of the fully coupled thermo-mechanical 3D model, usually treated under isothermal assumptions in the literature (eg. [2, 4]), is numerically implemented in the isogeometric analysis framework, a generalization of finite element method based on non-uniform rationalized B-splines (NURBS) basis functions [3, 5]. We conduct the new studies of microstructure evolution with hetrogeneous nucleation seed in the centre of a cube domain under the influence of mechanical loading. It has been found that the heterogeneous nucleation affects martensitic evolution morphology and promotes multivariant state near the vicinity of defect.

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Twinning in Strained Ferroelastics: Microstructure and Statistics

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The generation of functional interfaces such as superconducting and ferroelectric twin boundaries requires new ways to nucleate as many interfaces as possible in bulk materials and thin films. Materials with high densities of twin boundaries are often ferroelastics and martensites. In this review we show that the nucleation and propagation of twin boundaries depend sensitively on temperature and system size. Sudden changes of the domain pattern manifest themselves as avalanches or 'jerks' in the potential energy of the sample. At high temperatures, the change of the twin pattern is thermally activated, the probability, P, to find sudden energy changes of jerks E follows the Vogel-Fulcher statistics $P(E) \sim \exp(E/(T-T_{VF}))$, whereas the athermal regime at low temperatures corresponds to power-law statistics $P(E) \sim E^{-\varepsilon}$. We find that the complexity of the pattern is well characterized by the number of junctions between twin boundaries. Materials with soft bulk moduli have much higher junction densities than those with hard bulk moduli. Soft materials also show an increase in the junction density with diminishing sample size. The change of the complexity and the number density of twin boundaries represents an important step forward in the development of 'domain boundary engineering', where the functionality of the materials is directly linked to the domain pattern.

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Investigation on Temperature Uniformity in Thermo-diffusion Cells

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A thermodiffusion cell is used in conjunction with a Mach-Zehnder interferometer to measure properties of binary and ternary mixtures. In order to improve measurement accuracy to resolve subtle changes in the refractive index of a mixture in temperature gradient to be used to determine thermodiffusion properties, a new cell has been developed. This is a major improvement over the old cell design, which has been extensively used and proved sufficient in its range of application, Ref [1]. It can be shown that despite its acceptable capability, old cell design suffers from a number of shortcomings, which include non-uniform temperature distribution, limited measurement region due to poor thermal insulation, and misplaced injection points into the cell that cause disturbance during experiments. To study the current design and examine its limitations, a computational approach has been adopted. The numerical modeling results have led to an improved design that achieves uniform temperature distribution within the cell, improved insolation of the mixture from external thermal disturbances, and a radical approach to the injection of the mixture without disturbing the cell content. Furthermore, from the results of the computational approach, it is anticipated that the resolution and accuracy of the thermo-diffusion property measurements to be much increased.

To develop the new cell design, the natural convection heat transfer problem has been numerically modelled by choosing Boussinesq approximation. The cell is modelled to have a very small volume in a large medium (i.e., infinite domain approximation). This approach has been adopted for modelling both the new cell and old cell designs. The results are shown in Fig.1.

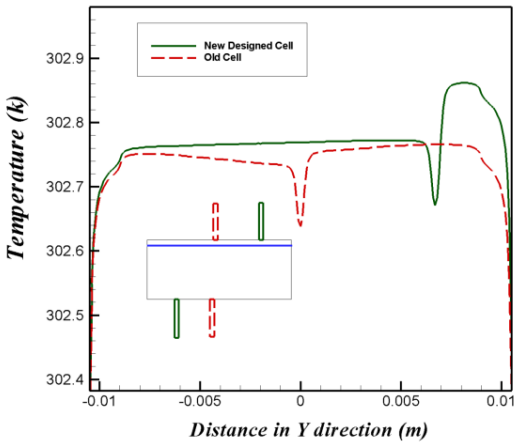

Figure 1: Temperature distribution on a horizontal line with 0.5 mm distance from top surface

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Non-equilibrium solidification in undercooled faceted-faceted Ni-56.2 Si at % eutectic alloy

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The maximum undercooling of 316 K was achieved in the bulk liquid Ni-56.2 at% Si eutectic alloy (faceted-faceted NiSi-NiSi2 eutectic alloys) melts through glass fluxing combined with cyclic superheating, in which a typical transition of faceted-faceted (FF) NiSi-NiSi2 eutectic takes place. A wide variety of microstructures can be obtained in the FF NiSi-NiSi2 eutectic alloys with the increase of undercooling. The metastable Si phase was obtained through slow post-solidification when undercooling $\geq$ 14 K, and it is confirmed by optical microscope (OM), scanning electron microscope (SEM) with an electron probe microanalysis (EPMA) and differential scanning calorimetry (DSC).

Based on the principle of minimum free energy and transient nucleation theory, the phase selection of melt was discussed with regard to the metastable phases formation in the bulk undercooled FF NiSi-NiSi2 eutectic alloys. In this paper, the formation of metastable phases from undercooled FF NiSi-NiSi2 eutectic alloys was determined by the competitive nucleation with undercooling, i.e., high undercooling facilitates the preferential nucleation of metastable phases.

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Homogeneous crystallization of Si_{136} clathrate from liquid: Molecular dynamics simulations

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Silicon clathrates are open-framework structures with slightly distorted tetrahedral coordinate. The materials based on the clathrates intercalated with gust species display interesting properties such as superconductivity[1], thermoelectricity[2] and high compressibility[3], thus attracting significant attention.

From the phase diagram of silicon, Si_{136} clathrate becomes stable thermodynamically in high negative pressure regime, which leads to great difficulty in synthesis. It is important to develop a feasible synthesis route to the new form of elemental Si. There are two approaches to achieve the goal up to now. The first method is the experimental removal of guest species from metal-doped clathrates[4], and the second one is the epitaxial growth proposed by molecular dynamics simulations[5]. However, the homogeneous nucleation (crystallization) of Si_{136} clathrate has not been observed in both experiments and simulations till now.

In this work, the guest-free Si_{136} clathrate is achieved by the homogeneous crystallization from liquid silicon using molecular dynamics simulations. The phase relations between the clathrate and the low density liquid (LDL) silicon are investigated at negative pressures below –2.0 GPa. The results indicate that the homogeneous crystallization of Si_{136} clathrate only occurs in a narrow pressure window from –3.60 GPa to –3.80 GPa. In the wide negative pressure regime above –3.60 GPa, liquid silicon preferentially transforms to LDL that is characterized by a local tetrahedral order. Such local ordered geometry favors the formation of diamond-structured silicon but suppresses the transition to Si_{136} clathrate. The influence of LDL tends to be eliminated with falling compressibility maxima as the pressure decreases, which allows for the observation of Si_{136} crystallization before liquid cavitation around –3.80 GPa. Upon compressing the Si_{136} clathrate above 800 K along isotherms, a transition to high density liquid Si is observed. Below 800 K, Si_{136} is found to be compressed into high density amorphous Si via two steps. The periodic arrangement of the cage-like clusters is destroyed firstly, and then the polyhedra are broken in the subsequent step. The present results provide a new pathway to investigate and prepare Si_{136} clathrates. It would be helpful to give an insight into the phase relations of silicon in negative pressure regime and explore the potential applications of clathrates.

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Analysis of twinned crystals via eigensymmetries of crystallographic orbits

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A *twinned crystal* (twin) is a heterogeneous crystalline edifice composed of two or more homogeneous crystals of the same phase with different orientation related by a twin operation t, i.e. a crystallographic operation mapping the orientation of one individual onto that of the other(s). The heterogeneity of twins forms an obstacle for the structural investigation and the technological applications of the concerned materials (e.g. the piezoelectric effect is reduced or annihilated by the presence of twinning). Material scientists growing crystals with targeted properties aim at avoiding the formation of twins. Understanding the formation mechanism is a 'condicio sine qua non' to develop a synthesis protocol capable of reducing, if not eliminating their occurrence. Our approach allows to obtain a general structural theory of twinning which gives the sufficient conditions for the formation of twins. It is based on the search for non-characteristic crystallographic orbits whose eigensymmetry contains the twin operation t.

Twins are based on the continuation, exact or approximate, of a substructure through the composition surface. The analysis of this structural continuity can be obtained by the analysis of the (pseudo)-eigensymmetry of the crystallographic orbits corresponding to occupied Wyckoff positions in the structure. Let $\mathscr{G}$ be the space group of the individual and O_i the orbits generated by the atoms of the structure under $\mathscr{G}$, with eigensymmetries $E(O_i)$ (as computed by the PSEUDO program [2]). The subgroup $\mathscr{H}$ of $\mathscr{G}$ which fixes the twin lattice is obtained as intersection of the space groups of the individuals in their respective orientations:

$$\mathscr{H} = \mathscr{G} \cap t\mathscr{G}t^{-1}.$$

By restricting the action to the subgroup $\mathscr{H}$, the atoms belonging to the orbit O_i are partitioned into a new set of orbits O_{ij} (split orbits) with eigensymmetries $E(O_{ij})$. The structural continuity is obtained if one of the following holds:
1) the (pseudo)-eigensymmetry of an orbit O_i contains the twin operation;
2) the (pseudo)-eigensymmetry of a union of orbits O_i contains the twin operation;
3) the (pseudo)-eigensymmetry of a split orbit O_{ij} contains the twin operation;
4) the (pseudo)-eigensymmetry of a union of split orbits O_{ij} contains the twin operation.

The case of the three known twins – (100), (001) and $(1\bar{2}0)$ – in melilite silicate (see [1, 3]) is analyzed and the quasi-restored orbits are illustrated. In particular, it is shown that the first two twins, which are indistinguishable from a lattice viewpoint (because the lattice is entirely restored by the twin operation in both cases) have a significantly different degree of structure restoration, which leads to an expected higher occurrence frequency for the (001) twin.

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Task Based Parallelization of Molecular-Dynamics Simulations with Short-Range Forces

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Molecular-dynamics simulations are a versatile tool that is widely used in computational materials science [1, 2]. For simulations with short-ranged forces, the standard approach to parallelization is spatial decomposition where each processor is responsible for particles in a subvolume of the simulated system [3]. An advantage of spatial decomposition is that it can be implemented on distributed systems as well as shared-memory machines. Furthermore, the approach scales well to large number of processors as long as there are enough particles on each processor to amortize the communication overhead and if the computational load is approximately the same on all processors.

In molecular-dynamics simulations of complex nanostructured materials or nanodevices it can be difficult to achieve a good load balance since in such systems the particles are often not homogeneously distributed in space. In order to overcome this problem a new approach is presented in this work. The calculation of the forces in the simulation is divided into small tasks. The tasks are dynamically assigned to a thread pool according to a dependent task schedule. The schedule ensures that two tasks that are running concurrently will never access the same particle. This procedure effectively eliminates the need for additional synchronization of particle updates. Although the method is designed for shared-memory machines, it integrates seamlessly into a hybrid scheme that uses message passing between nodes.

The task-based approach has been implemented in a modified version of a parallel molecular-dynamics code for large-scale simulations of materials [4]. Extensive tests of the parallel speedup have been performed for crystalline bulk copper, a spherical nanoparticle and a partially sintered, porous nanocrystalline material. Standard dual hex- and quad-core Xeon systems were used in the tests. In all cases the task-based approach achieves consistently high speedups. For crystalline copper, these speedups are comparable or slightly better than those achieved with spatial decomposition. For the other two systems, the task-based approach is clearly superior. Work is currently in progress to implement and test the new method on Intel's Many Integrated Core Architecture.

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Molecular Dynamics Simulation of Density for Undercooled Liquid Zirconium

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The molecular dynamics (MD) simulation has been extensively applied in materials science as a powerful approach[1], especially in exploring metastable liquids, and thus procucting novel materials. Zirconium is an important metal in nuclear reactors due to its low neutron absorption [2], and also in metallic glass formation. Unfortunately, the fundamental properties of liquid zirconium, such as density etc. are rather limited due to the great experimental difficulty, especially for metastable state. The objective of this work is to study the density dependance of temperature of liquid zirconium by MD method.

The developped embedded atom potential model [2] is applied to simulate a cell with 4000 atoms. Nose-Hoover's NPT algorithm is performed at 100 K temperature interval, in which 200000 steps are carried out for equilibrium and deriving the final results. The simulated density linearly increases with the drop of temperature, including a maxium undercooling of 928 K, as shown in Fig. 1. The density value is 6.00 g cm^{-3} at the melting point of 2128 K, and the temperature coefficient is -2.24×10^{-4} g cm^{-3} K^{-1}. Also, the results in previous literatures[3-5] are given in Fig.1. The present result shows the relationship between density and temperature in a much broader temperature range. Especially, the data are presented for the undercooling beyond 300 K, which have not reported in the available references. This work was financially supported by National Natural Science Foundation of China (Grant No.s 50971103, 51027005 and 51271150), the Program for New Century Excellent Talents of MOE, and China Scholarship Council.

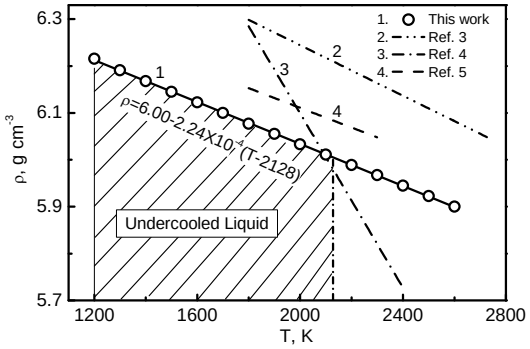

Figure 1: The density of stable and metasatable liquid zirconium versus temperature.

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Drilling Force and Temperature of Metalic Material with Hollow Drill

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Drilling force and temperature must be controlled during the drilling of workpiece. Most of the existing literatures proposed experimental methods to reduce drilling force and detect temperature with twist drills. In some occasions, the hollow drill is required to implement drilling in stead of twist drill or core drill. In some sense, finite element analysis could provide useful data with proper computational algorithm and accurate model before designing experiments [1-3]. The drilling simulation could efficiently decrease the cost spent on experiments and uncertain risk.

In this talk we studied the difference of drilling force and temperature between hollow drill and twist drill. The simulation was performed in Deform 3D which generated the model of workpiece with a hollow drill model from Solidworks (seeing Figure 1). The metalic material models of hollow drill (Carbride-15%Cobalt) and workpiece (Al-20%Si_s_machining) were imported from the material library. The stress, strain, velocity, temperature and deformation of the drilling process were obtained in the defined number of simulation steps. The force curves were drawn based on the computational results in post-process. The simulation results show that the drilling force rapidly increase before the drill tip entirely drilled into the surface of workpiece (seeing Figure 2) and the mesh of the drilling model has significant effect on computation. Furthermore, the variation of drilling force and temperature against rotational speed and feed rate are consistent with the references performed on twist drills [1-4]. This work is supported by the State Scholarship Fund of China (No.2011629094), Natural Science Foundation of China (NSFC: 51105316) and NPU Foundation for Fundamental Research (NPU-FFR-JCY20130118).

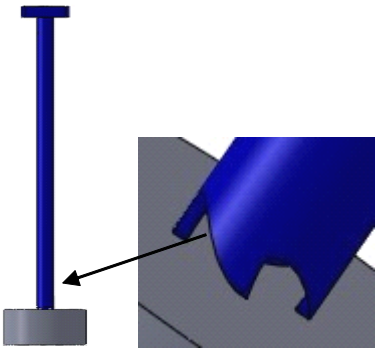

Figure 1: 3D models of howllow drill and workpiece.

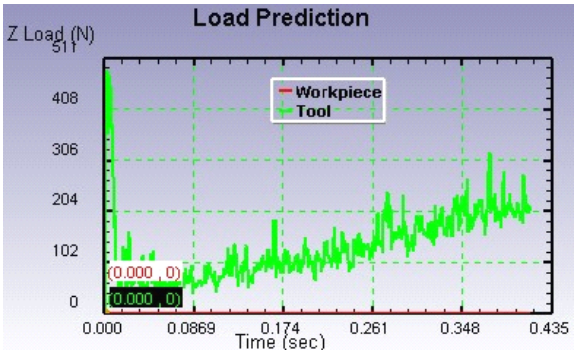

Figure 2: Drilling force curve.

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Hysterisis Algorithm For Alleviating Organic LED Degradation

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Development and application of novel materials, metallic alloys[1], inorganic and organic materials[2], have a increasing close relationship with computational science. Luminescent materials and its efficiency is becoming the most popular research domain in organic light emitting diode (OLED) devices. Fluorescence, compared to phosphorescence, has long lifetime, high thermostability and low fabrication cost. Recently, thermally active delayed fluorescence (TADF) material has been developed, which dramatically improves green and blue lighting efficiency [2]. However, the manufacturing process non-uniformity issue still causes unreliable performance even though high efficient lighting materials are applied in OLED devices. Currently, various driving schemes have been reported for minimizing ununiform brightness effect based on voltage [3] or current driving scheme and optical feedback scheme.

In this paper, a newly-elaborated compensation scheme is proposed for overcoming the problem of non-uniformity on ITO/CuPc/NPB/Alq_3/LiF/Al passive matrix OLED based on the interdependence between its luminance degradation and current drop under bias stress. The proposed method develops techniques of digital control algorithm with feedback iteration to program driving current fed into one OLED pixel within a certain hysterisis window according to the junction voltage increase in aging process. Charge bump and small detecting resistor are also adopted in the circuit to provide constant current source and detect pixel driving current, respectively. Figure 1 shows the simulation results that the compensation scheme can correspondingly add the extra current for the large impedance degraded OLED pixel in order to maintain the same brightness. This work is supported by Natural Science Foundation of China (NSFC: 51105316) and NPU Foundation for Fundamental Research (NPU-FFR-JCY20130118).

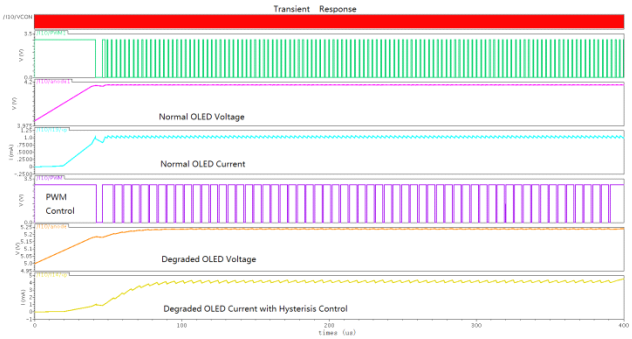

Figure 1: Transient simulation of normal and degraded OLEDs with hysteresis control and degradation compensation.

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Phase separation and dendritic growth of bulk undercooled ternary Co-Cu-Pb alloy

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As an important phase transformation phenomenon, phase separation is commonly observed in various condensed matter systems such as polymers, oxides and metallic alloys [1, 2]. Especially for metallic alloys, the phase separation process of immiscible alloy melts has attracted extensive research both theoretically and experimentally in relevant fields for several decades [3]. The dendritic growth within undercooled immiscible alloy melts has also drawn more and more attention due to its potential technological applications [4]. When bulk undercooling becomes large, the dendrite growth velocity is usually enhanced and the solidification kinetics is far from equilibrium condition. The related nonequilibrium effects have been studied by many researchers for binary alloys. Further investigations remain to be done on the phase separation and dendrite growth mechanisms of more complicated ternary immiscible alloys.

The phase separation and rapid solidification of liquid ternary $Co_{45}Cu_{42}Pb_{13}$ immiscible alloy have been investigated under both bulk undercooling and containerless processing conditions. The macrosegregation pattern of the undercooled bulk alloy solidified under glass fluxing condition shows a vertical two-layer structure, which is composed of a top Co-rich zone and a bottom Cu-rich zone. As a comparison, the containerlessly solidified alloy droplets in drop tube are mainly characterized by two or three-layer core-shell structures, where the Co-rich zone is located at droplet center and the Cu-rich shell surrounds the Co-rich core. The undercooling of bulk alloy varies from 30 to 112 K at the cooling rate of 11~18 K/s. In Co-rich zone, a structural morphology transition of α(Co) phase from a coarse dendrite to an equiaxed grain takes place with the increase of undercooling. Meanwhile, the growth morphology of α(Co) phase changes from globules to fine dendrites in Cu-rich zone. The dendritic growth velocity of primary α(Co) phase shows a power-law relation to undercooling and achieves a maximum of 1.52 m/s at the undercooling of 112 K. According to the theoretical calculations based on the dendritic growth model, the growth of primary α(Co) phase is mainly controlled by solute-diffusion and the solute trapping occurs under high undercooling conditions. Numerical analyses indicate that the Stokes motion, solutal Marangoni convection, thermal Marangoni convection and interfacial energy play the main roles in the correlated process of macrosegregation evolution and microstructure formation.

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Computational Photonics (SS-CPH)

Organizers:
Marek Wartak (Wilfrid Laurier University)
Harry E. Ruda (University of Toronto)

This emerging field of computational science is playing a critically important role in designing new generations of integrated optics modules, long haul transmission and telecommunication systems. An important part is played by studies of the behavior of light and light-matter interactions using analytical and computational models. Possible areas of applications include 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 photonics.

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Near and Far Fields in High Quality Resonances of a Periodic Grating

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Although the scattering of a plane wave by a periodic grating of circular cylinders is a fundamental problem of electromagnetics and has been profoundly studied since the 1960s [1], the direct notion of the specific resonances appearing near Rayleigh "anomalies" appeared only recently [2]. Late we have proven that these resonances are associated with so-called "grating modes" as specific poles of the field as a function of frequency [3]. For sub-wavelength cylinders, these poles always cluster near the Rayleigh anomalies or, in other words, their frequencies depend mainly on the grating period.

We have comprehensively investigated an infinite grating, having the period p, of identical parallel circular dielectric cylinders with radius a and refractive index α. The grating has been studied as a scatterer and also as a resonator that implies an eigenvalue problem. In the first case, we look for the reflectance of the normally incident plane wave and the field in the near and far zones. In the second case, the eigenvalues are sought in two different forms: firstly, as pairs of two real values: the lasing threshold or negative imaginary part of the cylinders' refractive index γ and real-valued frequency $\sigma = p/\lambda$ (λ being the wavelength) or, alternatively, in more classical way as complex frequencies. Accurate Maxwellian formulation and the casting of the problems to Fredholm second-kind matrix equations allow using the Gershgorin theorem for localization of the eigenvalues. On splitting the matrix by symmetry we obtain the following expression for the quality-factor of the first grating mode of the H-polarization, having $\sigma' \approx 1$:

$$Q = -\frac{\sigma'}{2\sigma''} = \frac{(\pi - 1)p^4}{2(\alpha^2 - 1)a^4\pi^4}, \tag{1}$$

and the inverse value for the lasing threshold γ. As one can see, the quality-factor the grating mode enhances as the grating gets sparser. This is not a trivial fact as the volume of the resonator gets smaller. As we see in Fig. 1, for the grating parameters $p/a = 10, \alpha = 2.48$ the near field in such resonance is dominated by an intensive standing wave along the grating, stretching very far in the normal direction. This shape becomes even more pronounced for larger values of p/a. By this reason the grating resonances can be viewed as the most promising physical effect for applications of periodic structures.

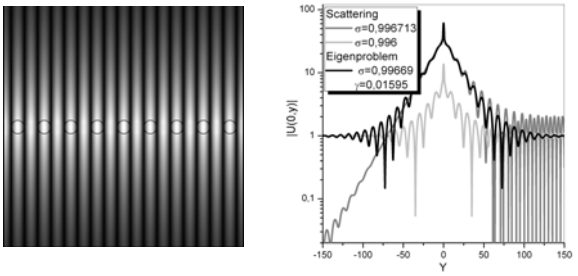

Figure 1: The total field magnitude and its cut along the normal to the grating for $p/a = 10$, $\alpha = 2.48$, $\sigma = 0.996713$.

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High order semi-Lagrangian solution of the Boltzmann-Poisson system: kinetic description of weakly collisional plasma.

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The Convected Scheme (CS) is a family of semi-Lagrangian algorithms, most usually applied to the solution of Boltzmann's equation, which uses a method of characteristics in an integral form to project a moving cell (MC) forward to a group of mesh cells. In earlier work [1], a 4th-order version of the cell-centered CS was presented, which was based on applying an a-priori correction to the position of the MC after the ballistic move and prior to remapping to the mesh. Such corrections were calculated by means of a modified equation analysis applied to the continuity equation with a prescribed flow field. The resulting 4th-order CS showed a drastically reduced numerical diffusion, while it retained the desirable properties of the original scheme (i.e. mass conservation, positivity preservation, and simplicity). More recently [2], arbitrarily high order versions of the CS were designed, suited to the accurate solution of the Vlasov-Poisson system with minimum computational resources. For sufficiently smooth solutions on a periodic domain, this new scheme shows spectral convergence to the exact solution. Such a method was applied to the kinetic description of non-collisional plasmas, and validated against classical 1D-1V test-cases in both the linear and non-linear regimes, where it showed unprecedented phase-space resolution and virtually no numerical dissipation.

In this work we introduce the effect of elastic and inelastic collisions, and we model the resulting Boltzmann-Poisson system. Specifically, we investigate the formation of a planar plasma presheath in a weakly collisional plasma, and we compare the new 1D-2V results with simulation performed with early versions of the CS [3]. In order to properly model an absorbing wall, two alternative implementations are investigated: a periodic extension of the domain, which allows us to use FFTs, and a hybrid scheme which uses lower order polynomial interpolation in configuration space. In both cases, the solution shows a very sharp gradient in phase-space, at the wall and for low velocities ($v \simeq 0$); such a gradient becomes a discontinuity in the limit of vanishing collisionality, and it requires careful treatment. While being strictly mass conservative, the proposed scheme does not exactly conserve the total energy, sum of kinetic and potential energy, even in the non-collisional case and for a periodic domain. Hence, we study the effect of inexact energy conservation on the solution, and we investigate the role of the time-splitting error by comparing traditional Strang splitting with higher order algorithms, as in [4].

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Predicting Optimal Finite Field Strengths Leading to Most Precise Calculations of Nonlinear Optical Properties

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The finite field (FF) method is a straightforward and easy-to-implement technique used in quantum chemistry to model the nonlinear optical (NLO) properties of molecules. However, its well-known dependence on the range of field strengths at which calculations are performed can compromise its efficiency.[1] We use the FF method to calculate the static dipole polarizability (α), first and second hyperpolarizability (β and γ) for a wide range of organic molecules. Within this set of 120 molecules, with two steps of Richardson extrapolation and field sequences of common ratio less than two, the truncation error is reduced and maximum precision is obtained (as compared to computationally more demanding response theory calculations).[2,3] (See Fig. 1a.) For each molecule, depending on the level of theory applied, a region of field strengths could be highlighted that produces the most precise calculations. From the correlations between the optimal field strength and different molecular quantities, we developed a protocol to estimate the optimal field strength *a priori*. Among several molecular quantities tested, the maximum nuclear distance within the molecule was the best predictor of the optimal field strength for calculating γ (Fig. 1b). These findings are currently being extended to lower derivatives of energy (α and β) and different levels of theory.

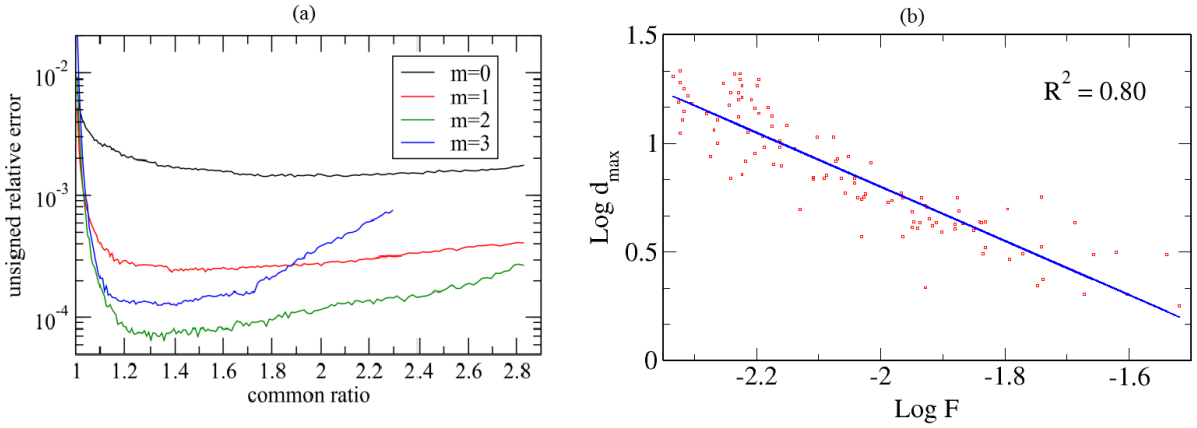

Figure 1: (a) The average minimal unsigned relative error of γ calculated for the 120 molecules of the data set at the HF/6-31G(d) level of theory as a function of the common ratio x and different steps of Richardson extrapolation m. (b) Correlation between the logarithm of optimal field strength for γ and logarithm of maximum nuclear distance.

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Mathematical and Computational Modeling of Noise Characteristics of Channel Amplifiers

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Microchannel electron multipliers, which amplify the input current of electrons through complicated stochastic processes, have found wide applications in different areas due to a number of remarkable properties [1]. However, statistical fluctuations in the gain of the channels increase a noise factor which is a measure of the loss of available information. Investigations dealing with reducing of the noise factor are of considerable practical interest.

This work is devoted to computational modeling of stochastic processes of the electron multiplication in the electron amplifiers in order to reduce the noise factor. Here, the effects of the processes, arising when a layer with increased secondary emission is formed at the entrance of the channel, are investigated. The following physical picture was considered in the modeling. The electrons of a parallel monochromatic beam entering the channel hit the walls at different incidence coordinates, producing secondary electrons which are multiplied until they leave the channel. The high-efficiency emitter is deposited on the top of the contact conducting layer. Since there is no potential drop along the conducting layer, the conditions for the movement of secondary electrons in this region are different from motion of electrons in a uniform field inside the channel. Due to the spread in the collision coordinates the input electrons bombard the high-efficiency emitter and the wall of the channel not coated with the high-efficiency emitter. The area covered by the input electron beam depends on the incidence angle of the primary electrons. All these factors and parameters are taken into account in the model.

A computational method for simulation of stochastic processes of an electron multiplication in microchannel electron amplifiers is developed. It is based on 3D Monte Carlo (MC) simulations and theorems about serial and parallel amplification stages [2]. Splitting a stochastic process into a number of different stages, enables a contribution of each stage to the entire process to be easily investigated. The method preserves all advantages of the MC simulations which are used only once for one simple stage. The use of the theorems allows to conduct any further investigations and optimizations without additional MC simulations. The method provides a high calculation accuracy with minimal cost of computations. The nonuniform field at the entrance of the channel is calculated by the finite difference method for the Laplace equation. The part of the channel with nonuniform field is considered as a separate stage. The trajectories of the electrons in the nonuniform field are calculated by the Runge-Kutta method.

The method is used to investigate the effect on the noise factor of the incidence angle and energy of the input electron beam, the spread in incidence coordinates of the primary electrons, nonuniformity of the emitter surface, the length of the contact conducting layer, and the depth and secondary emission yield of a high-efficiency emitter. All these investigations are done without additional MC simulations for the same channel geometry. The model easily implements new experimental data without any changes in the algorithm.

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On the numerical solution of chromatographic separation models

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In a chromatographic separation model one has several species moving in a fluid and interacting with each other. For each species there are 3 different variables: concentration of the liquid phase C, concentration of the solid phase S and equilibrium concentration in the interface between 2 phases E. In addition we have the vector field describing the fluid flow but this is supposed to be known.

If we have k species the model has k convection diffusion equations for C, k ODE for S and finally k constraints or algebraic equations relating C and E. The numerical difficulty of solving this kind of system is due to the fact that the algebraic equations are highly nonlinear. The standard approach has been to design special numerical schemes which would preserve the constraints as well as possible. Here we take a different approach. We differentiate the constraint equations to obtain genuine dynamics also for E variables. However, we do not forget the algebraic constraints and treat the whole system as an overdetermined problem.

One might say that in the standard approach one tries to keep the system simple and one has to design complicated numerical schemes while in our approach we make the system a bit more complicated but then we can use any standard methods for PDE. The advantage is thus that this methodology is not dependent on the particular form of the system.

We illustrate our approach using a 2 species model where one species is the salt and the other a certain protein. In this case one can actually visualize the constraint manifold as a surface in R^3. Nonlinearities are indeed very strong but the manifold itself is not geometrically complicated. Hence there is no reason why the problem should be intrinsically numerically complicated. Indeed our computations show that with our modified model one obtains good results with standard numerical methods.

Computations in Systems Biology (SS-CSB)

Organizers:
Hin Hark Gan (NYU)
Gaurav Arya (UCSD)

Systems biology is the study of complex interactions within cells and how such interactions lead to emergent biological phenomena. This session explores recent progress in the development and application of computational methods towards the understanding of cellular processes and phenomena such as transcriptional and translational regulation, epigenetics, cell signaling, and diseases. The focus will be on assessing the efficacy of biophysical, bioinformatics and mathematical approaches for understanding current experimental data.

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Accelerated molecular dynamics simulations and community network analysis reveal allosteric signaling pathways in a lectin-binding chaperone Calreticulin

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Calreticulin (CRT) is a multi-domain lectin-binding chaperone that plays an important role in the assembly and folding of the major histocompatibility complex (MHC) class I molecules that present antigenic peptides on the cell surface and enable their recognition by T-cells. Specifically, CRT binds to both specific oligosaccharide structures on MHC class I molecules during their folding as well as a polypeptide part of MHC and thus plays a crucial role in stabilizing folding intermediates, preventing aggregation, and allowing the MHC protein to attain its native structure. Recent experimental studies have shown that the initial interaction between CRT and a monoglucosylated MHC protein is glycan-driven (i.e., interaction occurs through oligosaccharides), with glycan-independent interactions representing a second step in the chaperone cycle of CRT. Still, what factors trigger a switch from glycan-dependent to glycan-independent mode of interactions between CRT and its substrate is not well understood. Through computational investigations involving molecular dynamics simulations and structure based molecular docking as well as collaborative experimental studies with Raghavan group we have shown that ATP-binding serves as a switch for toggling CRT between two distinct modes of interactions. Specifically, our results show that binding of ATP on CRT at the location that is distant from the glycan binding site leads to reduction in the affinity of CRT toward glycans and thus acts as a switch that induces a disengagement of a glycan from CRT, and induces exposure of hydrophobic regions on the surface of the globular domain allowing CRT to act as a chaperone through favoring interactions with the polypeptide component of the MHC. Further, employing accelerated molecular dynamics simulations of CRT bound to glycan and ATP together with community network analysis derived from molecular dynamics we have predicted residues that participate in allosteric signaling between ATP and glycan binding site of CRT. Modifying these residues has a large effect on the communication pathways in CRT consistent with experiments and support our model of ATP as a switch for CRT function.

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3-D Higher-Order Folded Chromosome Conformations From 2-D Interaction Frequency Maps

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Chromatin is a fiber of histone proteins and DNA present in the nuclei of eukaryotic cells. The higher-order folding of chromatin into chromosomes, which affects various genomic processes ranging from transcription to recombination, has so far remained elusive. Recently, sophisticated experimental techniques, collectively known as chromosome conformation capture (3C), have been developed to measure the frequencies of interaction between different DNA segments within and across chromosomes [1, 2]. Such 2D maps of interaction frequencies (IFs) can in principle be used to deduce the 3D higher-order folding of the chromatin fiber, though this is a highly challenging computational problem. Here, we present a new computational approach [3] to recover the ensemble of chromatin conformations consistent with a set of given IF measurements. In this approach, we treat the examined chromosomal domain using a restrained bead-chain model, which captures the physical properties of the chromatin fiber and its looping interactions. We then perform dynamical simulations of such a restrained bead-chain to determine its ensemble-averaged IF map and utilize an adaptive learning algorithm to iteratively refine the strengths of the imposed restraints until a match between the computed and input IF map is achieved. Our approach offers multiple advantages over existing alternatives, including use of physical models of chromatin, avoidance of preconceived relationships between IFs and spatial distances, prediction of ensembles rather than unique structures, and intrinsic validation of the computed ensemble based on IF. The above approach has been validated against multiple simulated test systems, and we are currently refining the approach against known experimental IF and spatial distance measurements. We expect the final, refined approach to become a valuable tool for researchers examining the higher order organization of chromatin.

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Mechanics of microRNA-mediated translational regulation

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Current computational analysis of microRNA interactions is based largely on primary and secondary structure analysis. Computationally efficient tertiary structure-based methods are needed to enable more realistic modeling of the molecular interactions underlying miRNA-mediated translational repression. We incorporate algorithms for predicting duplex RNA structures, ionic strength effects, duplex entropy and free energy, and docking of duplex-Argonaute protein complexes into a pipeline to model and predict miRNA-target duplex binding energies. To ensure modeling accuracy and computational efficiency, we employ an all-atom description of RNA and a continuum description of ionic interactions using the Poisson-Boltzmann equation. Our method predicts the conformations of two constructs of *Caenorhabditis elegans let-7* miRNA-target duplexes to an accuracy of ~3.8 Å root mean square distance of their NMR structures. We also show that the computed duplex formation enthalpies, entropies and free energies for eight miRNA-target duplexes agree with titration calorimetry data. Analysis of duplex-Argonaute docking shows that structural distortions arising from single base pair mismatches in the seed region influence the activity of the complex by destabilizing both duplex hybridization and its association with Argonaute. Collectively, these results demonstrate that tertiary structure-based modeling of miRNA interactions can reveal mechanisms not accessible with current secondary structure-based methods. Future work integrating 2D- and 3D-based methods should allow transcriptome-wide analysis of post-transcriptional regulation mediated by miRNAs.

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Genome organisation influences cell type-specific transcriptional programs

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The objective of our research is to understand how gene expression programs are regulated in a cell type-specific and developmentally regulated manner. Recently, chromatin looping has emerged as an important regulatory mechanism that brings distal enhancers into close physical proximity to the genes they regulate. In fact only 7% of distal enhancers in the human genome appear to regulate the closest gene in the linear sequence [1] and they therefore require chromatin loops to contact the gene(s) they regulate. In addition to chromatin loops allowing contact between distal enhancers and gene promoters, co-expressed genes are recruited to shared transcription permissive nuclear compartments when transcribed [2]. This recruitment is non random, can occur for genes on the same or different chromosomes, and depends on co-regulation by specific transcription factors [3, 4]. At a whole genome scale entire chromosomes occupy distinct territories in the nucleus which have been observed to intermingle along their boundaries by DNA FISH (fluorescence in situ hybridization) although the functional significance of this intermingling is not well understood.

To investigate genome organisation and gene transcription we use a combination of cellular imaging-based single cell assays (RNA FISH, DNA FISH, and immunocytochemistry) and cell-population based whole genome RNA sequencing (RNA-Seq) and chromosome conformation capture (3C, 4C, Hi-C). As pluripotent embryonic stem (ES) cells are known to have unique chromatin features which are lost at the very early stages of differentiation they are an ideal system in which to study dynamic changes in genome organisation and gene transcription. By interrogating Hi-C data from published studies [5,6] we observed that interactions between different chromosomes can account for 50% of a sequenced Hi-C library, however, both human and mouse ES cells display substantially fewer (10-15%) inter-chromosomal interactions than differentiated cell types suggesting that chromosomes intermingle to a lesser degree in these cells. In all cell types investigated, both common and unique chromosome pairing preferences were observed in the Hi-C data. Chromosome pairs were chosen based on the Hi-C data and investigated by DNA FISH. Pairs chosen for their close nuclear proximity based upon Hi-C interaction data were used to ascertain that the chromosome territories of these pairs within ES cells are significantly further apart than they are within differentiated cells. These data highlight the conformity between the molecular data of Hi-C and single cell imaging studies. Intriguingly these data also reveal that individual chromosome territories intermingle to a lesser degree in ES cells which may play an important role in maintaining the pluripotent phenotype or be a result of the increased transcriptional activity observed in ES cells.

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Investigating Oscillatory Phenomena in the Continuous Bioreactor for Production of Bioethanol Using Zymomonas Mobilis

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A mathematical model is built to investigate the oscillatory behavior in the continuous stirred bioreactor for producing bio-ethanol using Zymomonas mobilis yeast. It is found that the feed substrate concentration plays an important role for the occurrence of periodic behavior at low dilution rates. The oscillatory behavior dominates the system in the range of feed substrate $[70-245]g/L$ at $d = 0.05h^{-1}$. It is found that one of the proposed solutions to remove the oscillations is to increase the dilution rate. The periodic and stationery solutions are investigated in a wide range of feed substrate concentrations using bifurcation analysis and non-linear dynamics. It is found that at a high feed substrate concentration $C_{SO} = 220g/L$, and a high value of $d = 0.078h^{-1}$ which is greater than that used in the periodic phenomena, the stationery stat dominates the fermentation system, however, the oscillatory behavior appears again when the dilution rate is lower than 0.05. Furthermore, the period doubling dominates the system in the range of $d[0.028-0.0086]h^{-1}$ which is considered as the main way leading to chaotic behavior.

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Translational Systems Biology: understanding the limits of animal models as predictors of human biology

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Inferring how humans respond to external cues such as drugs, chemicals, viruses or hormones is an essential question in biomedicine. Very often, however, this question cannot be addressed due to the impossibility to perform experiments in humans. A reasonable alternative consists of generating responses in animal models and "translating" the results to humans. The limitations of such translation, however, are far from clear, and systematic assessments of its actual potential are badly needed.

We designed a series of challenges in the context of the 'sbv IMPROVER' project (Industrial Methodology for Process Verification in Research; http://sbvimprover.com/) to address the issue of translatability between humans and rodents. Our main aim was to understand the limits and opportunities of species to species translatability at different levels of biological organization: signalling, transcriptional, and release of secreted factors (such as cytokines, chemokines or growth factors). To address this question, we selected Normal Bronchial Epithelial Cells from both human and rat origin. These cells were exposed to 52 different substances and for each stimulus, samples were collected at different time points to generate phosphoproteomic, gene expression and secreted protein data.

The central questions we posed in this challenge were:

- Can the phosphoproteomic responses induced by stimuli addressing several distinct signalling pathways in human cells be predicted given the responses generated with the same stimuli in rat cells?
- Which gene expression regulatory processes (biological pathways / functions) are translatable and therefore predictable across species, and which are too divergent?

Summarizing, we presented the community with questions and data aimed at assessing methodologies designed to infer human biology from non-human biology.

The sbv IMPROVER project, the website, and the Symposium are part of a collaborative project designed to enable scientists to learn about and contribute to the development of a new crowd sourcing method for verification of scientific data and results. The project team includes scientists from Philip Morris International's Research and Development department and IBM's Thomas J. Watson Research Center. The project is funded by PMI.

Dynamics and Bifurcations in Coupled Networks of Differential Equations: Theory and Applications (SS-DBCNDE)

Organizer:
Luciano Buono (University of Ontario Institute of Technology)

The study of coupled networks of differential equations is a rich field of research having experienced recent theoretical advances and displaying a vast array of applications in physics and biology, amongst others. This special session will bring together researchers from various backgrounds who are actively involved in the study of dynamics and bifurcations in coupled networks. The scope of the session will be broad, with theoretical and applied contributions including coupled networks of ordinary differential equations, delay-coupled differential equation systems and networks with random coupling.

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Low-dimensional descriptions of neural networks

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Biological neural circuits display both spontaneous asynchronous activity, and complex, yet ordered activity while actively responding to input. When can model neural networks demonstrate both regimes? Recently, researchers have demonstrated this capability in large, recurrently connected neural networks, or “liquid state machines", with chaotic activity [1, 2]. We study the transition to chaos in a family of such networks, and use principal orthogonal decomposition (POD) techniques to provide a lower-dimensional description of network activity.

We find that key characteristics of this transition depend critically on whether a fundamental neurobiological constraint — that most neurons are *either* excitatory or inhibitory — is satisfied. Specifically, we find that constrained networks exhibit the transition to chaos at much higher coupling strengths than unconstrained networks.

This property is the consequence of the fact that the constrained system may be described as a perturbation from a system with non-trivial symmetries. These symmetries imply the presence of both fixed points and periodic orbits that continue to act as an organizing center for solutions, even for large perturbations. In comparison, spectral characteristics of the network coupling matrix [3, 4] are relatively uninformative about the behavior of the constrained system. In this talk, we will demonstrate this phenomena in a model network and investigate its impact on the ability of constrained networks to reproduce learning tasks that have been recently investigated in unconstrained networks [2, 5].

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Instabilities in delayed regulatory loops of the haematopoietic system

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The production of human blood cells is regulated through a highly complex, coupled set of feedback mechanisms involving, among others, differentiation of cell lines from a common pool of stem cells and hormonal interactions between circulating cells and cells at different stages of maturation [3]. As part of a global modeling project of the full haematopoietic system, and its perturbation under pharmaceutical interventions such as chemotherapeutic treatments, we consider the prototypical system of two coupled, negative feedback loops with time delays given by

$$\begin{aligned} \frac{dx}{dt} &= -\alpha x + f_1(x(t-\tau_1)) + f_2(y(t-\tau_2)) \\ \frac{dy}{dt} &= -\beta y + g_1(x(t-\tau_1)) + g_2(y(t-\tau_2)) \end{aligned}$$

where the functions f_i and g_k, which are monotone decreasing in each of their arguments, are taken as Hill's functions. This caricature system mimics the juxtaposition and interaction in the production of erythrocytes (red blood cells) and thrombocytes (platelets), these species being predominantly regulated by, respectively, erythropoietin and thrombopoietin. Our interest revolves around clinical observations at low levels of either of the hormones and their effective replacement by the other in supporting production of the respective cell line [1, 2]. Stability analysis of the equilibrium solution, which is shown to be unique, and computer-assisted centre manifold computations are used to determine the nature of, and the regulatory rôle played by, Hopf bifurcations in this system of delay-differential eqautions.

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Network synchronization and mixed couplings: when friends turn enemies and vice versa

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This talk discusses the influence of network structure on synchronization in dynamical networks with mixed graphs. A mixed graph is composed of subgraphs, connecting a subnetwork of nodes via one of the individual oscillator's variables. An illustrative example is a network of Lorenz systems where some of the nodes are coupled through the x-variable, some through the y-variable, and some through both.

We extend the connection graph method [1, 2] to derive bounds on the synchronization threshold in diffusive networks with mixed linear couplings and show that such mixed networks can have drastically different synchronization properties from networks connected through the same variables. More specifically, we prove that replacing a lightly loaded link with a stronger converging coupling via another variable (for example, replacing an x- with a y-coupling link in a network of coupled Lorenz systems) can improve synchronizability. However, such a replacement of a highly loaded (bottleneck) link can essentially worsen synchronizability and make the network unsynchronizable.

We also discuss synchronization of bursting neurons [3, 4] with mixed excitatory and inhibitory connections. Fast inhibition is known to promote pairwise asynchrony in inhibitory bursting networks [4]. We show that the addition of such repulsive inhibition to excitatory networks induces bursting synchrony, in contrast to one's expectations. Through stability and geometrical analysis, we reveal the mechanism underlying this purely synergetic phenomenon and show that it originates from the transition between bursting of different types caused by excitatory-inhibitory synaptic coupling [5].

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A Network of Symmetrically Coupled Gyroscopes

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Traditional gyroscopes are mechanical devices used for measuring and maintaining orientation. They consist of spinning discs enclosed in gimbal rings that allowed for free rotation in any orientation. While accurate, these purely mechanical sensors are limited in application due to their size and friction wear. New manufacturing techniques in microelectromechanical systems (MEMS) allow for mass manufacturing of low-cost and miniaturized vibratory gyroscopes. Given their size and price, these MEMS gyroscopes are commonly found in modern electronics. At the same time, these smaller gyroscopes are more prone to external perturbations. Small disturbances, such as thermo interference, can increase phase drifts in the oscillatory signal and give inaccurate results. Thus, these gyroscopes do not meet the more rigorous requirements for use in guidance systems.

To remedy the lowered sensitivity problem, researchers are considering networks of coupled MEMS gyroscopes. Experimental [3] and numerical studies [1, 2, 4] showed that networked MEMS gyroscopes can increase the sensitivity while minimizing phase drift. In this work, we continue the previous studies by using analytic methods on a network of symmetrically coupled gyroscopes in a Hamiltonian setting. We first investigate the effects of various coupling schemes on the Hamiltonian array. Then, we apply group theoretic and normal form techniques to simplify the system. Equations of motion of the reduced system are obtained. Synchronization behavior from bifurcation and numerical analysis of the simplified system are also presented.

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Emergent Collective Behaviour on Stochastic Coupled Cell Networks

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We consider stochastic dynamical systems defined on networks that exhibit the phenomena of collective synchronization and metastability; by this we mean network dynamics where the individual nodes' dynamics are typically quite simple, but that the configuration exhibits complicated dynamics in its collective behavior. For concreteness, we concentrate on the case of SDE defined on networks. We also present some specific results relating to stochastic perturbations of the Kuramoto system of coupled nonlinear oscillators. Along the way, we will observe a non-standard spectral problem appearing in all of these calculations, and see that the important features of this spectral problem are related to a certain homology group defined only by the network's topology.

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Chaos and reliability in fluctuation-driven, balanced spiking networks

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The question of reliability arises for any dynamical system driven by an input signal: if the same signal is presented many times with different initial conditions, will the system entrain to the signal in a repeatable way? In particular, this concept of the reproducibility, or reliability, of stimulus-induced activity has a long history in neuroscience [1, 2]. Of particular interest are large, randomly coupled networks of excitatory and inhibitory units which reproduce the irregular firing that typifies cortical activity. Several models of neural dynamics are known to autonomously produce strongly chaotic dynamics, with extremely strong sensitivity of spike outputs on tiny changes in a network's initial conditions [4, 3, 5]. Here, we show that such chaos also occurs in the presence of weak and strong stimuli [6]. However, even in the chaotic regime, intermittent periods of highly reliable spiking often coexist with unreliable activity.

We propose a framework to better understand these complex dynamics, leveraging results from random dynamical systems (RDS) theory, by establishing the effect of the underlying time-dependent chaotic attractor's geometry on output spike trains. We elucidate the local dynamical mechanisms involved in this intermittent reliability, and investigate the relationship between this phenomenon and the Lyapunov exponents spectrum arising from the dynamics. A conclusion is that chaotic dynamics do not have to be an obstacle to precise spike responses, a fact with implications for signal coding in large networks.

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Reduced Dynamics and Noise Stabilization for Stochastic Delayed Systems.

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The analysis of nonlinear delay-differential equations (DDEs) subjected to external forcing is difficult due to the infinite dimensionality of the space in which they evolve. To simplify the analysis of such systems, we first develop a non-homogeneous center manifold (CM) reduction scheme, which allows the derivation of a time-dependent order parameter equation in finite dimensions [1]. This differential equation captures the major dynamical features of the delayed system. The forcing is assumed small compared to the amplitude of the autonomous system, in order to cause only small variations of the fixed points and of the autonomous CM. The time-dependent CM is shown to satisfy a non-homogeneous partial differential equation. We show, for the general scalar case, how an ansatz separating the CM into a part for the autonomous problem plus a time-dependent order-two correction leads to satisfying results. We apply the method to a transcritical bifurcation with a single or multiple periodic forcings, and highlight the validity limits of the reduction scheme. This easily leads to the case of additive stochastic driving, which we illustrate for the transcritical bifurcation. Here additive white noise shifts the mode of the probability density function of the state variable to larger amplitudes.

We further present a stochastic bifurcation in a system wth pitchfork bifurcation in the presence of both delay and additive noise [2]. A stochastic center manifold method can compute a non-delayed stochastic order parameter equation for a scalar delayed system driven by additive uncorrelated noise. This is the first analytical demonstration of noise induced transitions in such scalar SDDEs. The derived order parameter equation includes additive and multiplicative white and coloured noise. An illustrative neural system with delayed self-excitation reveals stationary states that are postponed by combined additive noise and delay. A nal brief analytical treatment of the derived order parameter equation reveals how the shift of the stationary states depends on the delay and the noise strength.

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Bifurcations of Networks of Heterogeneous Two-Dimensional Integrate and Fire Neurons

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Mean-field analysis is a process which reduces a large network of coupled oscillators into a smaller set of meaningful differential equations which are vastly simpler to analyze. Mean-field systems have recently been derived for networks of two-dimensional non-linear integrate and fire neurons [1]. Models in this class are able to realistically model the electrophysiology and action potential generation for many real neurons. The mean-field systems derived in [1] assumed homogeneity of these neurons. Here, we extend the homogeneous mean-field system in order to analyze networks of heterogeneous neurons. In particular, a set of mean-field equations is derived for a heterogeneous network. Bifurcation analysis is performed on the mean-field system to analyze how a heterogeneous network of Izhikevich neurons with spike frequency adaptation transitions to bursting, from tonically firing. The bifurcation types and regions can differ substantially in the heterogeneous case when compared to the homogeneous case. Other applications of the heterogeneous mean-field system of equations are discussed.

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Collective Behavior of a Network of Spin Torque Nano-Oscillators

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The 2007 Nobel prize in Physics was awarded jointly to Albert Fert and Peter Grunberg for their discovery of the Giant Magnetoresistance Effect (GMR). This effect is observed as a significant change in the electrical resistance of some materials depending on whether the magnetization of adjacent ferromagnetic layers are in antiparallel or in parallel. The most common application of this effect is the *spin nano-valve* device [2], which consists of at least two layers of ferromagnetic materials separated by a nonmagnetic metal layer. In one layer the magnetization vectors are fixed while on the other they are free. As predicted by Slonczewski and Berger [1, 4], a spin-polarized current can exert a torque on the magnetization of a ferromagnetic layer leading to precession. Then the GMR effect can convert the magnetic precession into microwave voltage signals and turn the valve into a *Spin Torque Nano-Oscillator* (STNO) whose power output, about 1 nW, is small. To generate a more powerful signal, several groups [2, 3] have proposed to harness the power of several STNOs connected together, see Fig. 1, but their collective behavior, which belongs to the field of nonlinear dynamics, has never been studied.

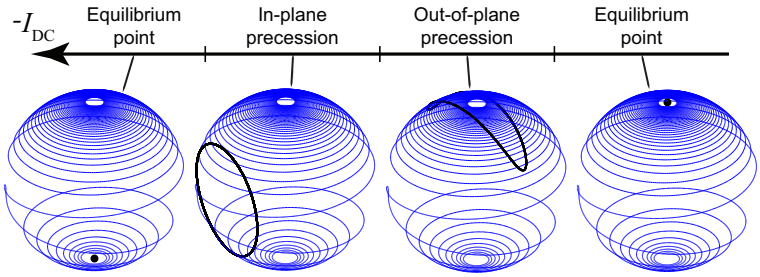

Figure 1: Collective behavior of two STNOs coupled in a series array through an external electrical current I_{DC}.

A typical network configuration with N nano-oscillators, connected in series, leads to a system of differential equations with all-to-all coupling. Thus, S_N–the group of permutations of N objects–is the underlying group of symmetries of the network. In this work we use ideas and methods from Equivariant Bifurcation Theory, in particular, Equivariant Hopf bifurcation with S_N-symmetry, to explore in more detail the collective behavior of the network and, in particular, to study the nature of the bifurcations that lead into and out of the synchronization state.

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Inducing Chaos in a gene regulatory network by coupling an oscillating dynamics with a hysteresis-type one

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In Gene Regulatory Networks, many regulatory processes are *homeostatic*, that is they maintain constant some viability parameters of an organism submitted to external perturbations.
Question: Is it possible to induce a disorder (that is, a chaotic behavior) in a homeostatic regulatory dynamics?

Homeostasis is usually caused by a negative feedback, that generates oscillations. In the case of a continuous modeling, these oscillations are often made by a *Hopf bifurcation*. To deal with our problem we consider a regulatory network of 4 genes called V-system, invented by J.J Tyson and E. Pécou, and modeled in order to couple in a very simple way a system admitting a Hopf bifurcation with a one having a *hysteresis-type dynamics*. Here are the 4 equations of this model:

$$\begin{cases} \dot{A_1} &= \dfrac{k_1 + k_{11}\left(\dfrac{A_1}{j_{11}}\right)^2 + k_{13}\left(\dfrac{A_3}{j_{13}}\right)^2}{1+\left(\dfrac{A_1}{j_{11}}\right)^2+\left(\dfrac{A_2}{j_{12}}\right)^2+\left(\dfrac{A_3}{j_{13}}\right)^2} - \gamma_1 A_1 \\ \dot{A_2} &= \dfrac{k_{21}\left(\dfrac{A_1}{j_{21}}\right)^2}{1+\left(\dfrac{A_1}{j_{21}}\right)^2} - \gamma_2 A_2 \\ \dot{A_3} &= \dfrac{k_3}{1+\left(\dfrac{A_4}{j_{34}}\right)^2} - \gamma_3 A_3 \\ \dot{A_4} &= \dfrac{k_4 + k_4\left(\dfrac{A_1}{j_{41}}\right)^2}{1+\left(\dfrac{A_1}{j_{41}}\right)^2+\left(\dfrac{A_3}{j_{43}}\right)^2} - \gamma_4 A_4 \end{cases} \tag{1}$$

We first use *slow-fast dynamics* to reduce the dimension of the V-system from 4 to 3, and then we show how to construct a *Smale's Horseshoe* in a general system having the same dynamical features as this system. This permits us to find conditions on the 17 parameters, for which the V-system approximately behaves as in this general case. We finish by showing numerical evidence that the mechanism creating chaos takes place in the V-system.

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Density Functional Theory (SS-DFT)

Organizer:
Ian Hamilton (Wilfrid Laurier University)
Paul Ayers (McMaster University)
Viktor Staroverov (Western University)

Density functional theory is a rapidly growing area of computational chemistry and physics. It is used for modelling the properties of materials ranging from atoms and molecules to clusters and nanostructures. In this minisymposium we focus on the development of mathematical methods to improve and extend the utility of density functional theory.

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Free energies of adsorption and activation energies for organo-arsenicals at the liquid/solid interface – a computational study.

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Methylated and aromatic arsenical compounds have various agricultural and industrial uses but once released into the environment they also become bio-available and a potential health hazard. The degree of mobility and bioavailability of these arsenical compounds depends highly on their interactions with reactive soil components. Thus, studying the mechanism of binding and calculating free energies of adsorption and activation energies for various reactions at the liquid/solid interface is useful for the development of accurate modeling tools as well as remediation technologies.

Herein, we present density functional theory (DFT) calculations for various ligand exchange reactions between organo-arsenical compounds and iron oxides with their Gibbs free energies of adsorption (ΔG_{ads}). Our studies reveal that both inner- and outer-sphere complexes form favorably with bidentate complexes being the most thermodynamically favorable. Single point energy calculations along reaction pathways are also included to show that high activation energies (~20 kJ/mol) are required to form bidentate complexes.

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Conceptual Density-Functional Theory Formulation of a General-Purpose Reactivity Indicator: Beyond the Classic Reactivity Paradigms

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Predicting how and whether two molecules will react is of fundamental interest in chemistry. Many molecules are most reactive either at the site with the largest charge (electrostatically-controlled reactions) or the site with the greatest electron transfer (Fukui-controlled reactions). But some molecules fall between these two paradigms. It is also frequently observed that only a few sites in a molecule are reactive and that the characteristic reactivity of these sites persists for a wide variety of incoming reagents [1]. As such one suspects that most of the details of the incoming molecule can be neglected. With these observations in mind one can construct a reactivity indicator by studying the molecular response to a simplified "model reagent" that mimics the charge and Fukui effects of the incoming molecule [2]. It is desirable that such an indicator is easily computable and conceptually accurate. The proposed indicator can be computed easily from the charges at each site of the molecule and from the charges at each site of the molecule with one fewer electron (if the molecule of interest is a nucleophile) or one additional electron (if the molecule of interest in an electrophile). Charges can be computed with a wide variety of quantum chemistry packages including Gaussian, which is the program used in my study.

In this talk I will discuss the formulation, computational scheme, and results that come from using this model. In particular, the model will be applied to a number of systems where the reactive sites are difficult (or even impossible) to describe using conventional methods, including boraphenanthrenes, which are molecules where frontier orbital theory fails to predict the correct reaction products [3]. This method is also effective for ambidentate ligands (e.g., thiocyanate, nitrite, and sulfite) and for electrophiles with both hard and soft reactive centers (e.g., dimethyl carbonate, N-methyl-N-nitrosotoluene-p-sulfonamide) [4].

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Accurate *ab initio* spin densities

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For large molecular systems such as transition metal complexes, density-functional theory (DFT) became instrumental in theoretical studies of mechanisms in metal-mediated catalysis. Yet, the treatment of open-shell systems remains a challenge for DFT [1]. In addition to the difficult prediction of ground states from states of different spin, spin density distributions considerably depend on the approximate exchange–correlation density functional if transition metal complexes containing noninnocent ligands are considered. Especially, nitric oxide as an open-shell molecule endows a corresponding transition metal nitrosyl complex with a complicated electronic structure for which qualitatively correct spin densities are difficult to obtain within the standard Kohn–Sham formalism [2].
We present highly accurate spin densities for an iron nitrosyl complex which we have identified as a challenging system for DFT and standard electron correlation methods [3]. Our approach is based on the density-matrix renormalization group (DMRG) algorithm [4, 5, 6] and allows the treatment of active orbital spaces beyond the current limit of 18 electrons correlated in 18 molecular orbitals. Furthermore, the explicit reconstruction of a complete-active-space configuration-interaction-type wave function [7] provides insights into chemically interesting features of the studied molecules such as the distribution of α- and β-electrons in terms of Slater determinants, CI coefficients, and natural orbitals. The DMRG reference spin densities can be used to validate the accuracy of DFT spin densities and assess the quality of the restricted active orbital spaces.

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Constrained 1DM Algorithm with Fractional Occupations

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We developed a new algorithm for Hartree-Fock and Kohn-Sham density-functional theory (DFT) based on direct optimization of the energy as a functional of the one-electron reduced density matrix (1DM). This algorithm is designed to be efficient for calculations on systems with fractional occupation numbers and to allow arbitrary linear and nonlinear constraints on the 1DM to be imposed. This provides a relatively simple approach to constrained-DFT and partition-DFT problems. In addition, by directly optimizing the 1DM we may circumvent the convergence failures one commonly encounters when modeling small band-gap materials.

In our algorithm, we minimize the energy with respect to the 1DM, γ, subject to the N-representability constraints and normalization condition on the 1DM (See Refs. [1]). We impose these conditions using the method of Lagrange multipliers (See Eqn. 1). The basic Lagrangian used in our code is therefore of the form

$$\Lambda[\gamma,\mathbf{B},\mathbf{P},\mu] = E[\gamma] - Tr[\mathbf{B}(\gamma-\gamma^2-\mathbf{P}^2)] - \mu(N-Tr[\gamma]) \tag{1}$$

Additional constraints may also be imposed on the 1DM by adding additional terms to this expression. For example, we can minimize the energy of the water molecule when the population of the oxygen atom is constrained to have a specific value. We optimize the resulting Lagrangian by minimizing the norm of the Lagrangian using a nonlinear Newton-Krylov solver. To demonstrate the program, I will present DFT and Hartree Fock energies for water at several nuclear configurations in a variety of basis sets. We have also calculated energies of water with atomic constrained populations.

Our approach is implemented in the Horton electronic structure package, which is being jointly developed at Ghent University and McMaster University. In due time we hope to transform our current proof-of-principle implementation into a full-featured linear-scaling DFT program.

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Kohn-Sham effective potentials from density and correlated wavefunctions

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A common approach when constructing the Kohn-Sham effective potential of a many-electron system is to use only its corresponding density. This methodology, however, leads to some undesirable effects such as oscillatory nonphysical potentials and non-injective density-to-potential mapping in finite basis sets. In this contribution, we discuss an alternative approach in which not only the density of the system is utilized but also the wavefunction. The proposed algorithm is expected to be robust when tackling the density-to-potential mapping problem.

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Energy Decomposition Analysis with Occupation Constraints

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Under the Kohn-Sham density functional theory (DFT) framework, we studied the binding energy for diatomic molecules using constrained-DFT. The new algorithm is based on the direct minimization of the energy as a functional of the one-electron density matrix (1DM), γ. In the algorithm we use the method of Lagrange Multipliers (see Eq. (1)) to enforce the normalization condition and the N-representability constraints on γ, as follows

$$\Lambda[\gamma, \mathbf{B}, \mathbf{P}, \mu] = E[\gamma] - Tr[\mathbf{B}(\gamma - \gamma^2 - \mathbf{P}^2)] - \mu(N - Tr[\gamma]) \tag{1}$$

This algorithm allows to impose linear and non-linear constraints to the 1DM, for example, to set the population of an specific atom **a** in a molecule,

$$Tr[\mathbf{P}_a \gamma] = N_a[\gamma] \tag{2}$$

were N_a is the number of electrons you are restricting into the atom **a**. We add these constraints to the Lagrangian (1) and then use a non-linear Newton-Krylov solver to minimize the norm of the resulting Lagrangian. This method brings a new approach to solve constrained-DFT problems, such as DFT energy decomposition analysis (EDA, see Ref. [1]). In the present work, we imposed population constraints (see Eq. (2)) to build the different bond cases, *i.e.* standard, covalent and ionic cases, hence we calculated the potential energy surfaces of a set of diatomic molecules for each case.

This algorithm is developed and integrated into the Horton electronic structure package, ensemble at University of Ghent and McMaster University.

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Variational Hirshfeld Ensemble

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It is common to exploit the one-particle electron density to partition a molecular system into atomic regions. The necessity for such a partitioning scheme is rooted in the unquestionable role of atoms in chemistry. Nevertheless, it is not well-defined concept within the domain of quantum mechanics, as it is not an observable. This has resulted in a proliferation of different approaches to retrieve the concept of atoms in molecules (AIM) within the domain of quantum mechanics and in silico experiments based on various flavours of model theories.

One of the popular families of models is the Hirshfeld partitioning scheme [1, 2]. In order to extend it, I have developed a variational version of Hirshfeld atoms with accurate electrostatic potentials; it aims to find the promolecular density that resembles the true density as much as possible. The key definition of Hirshfeld-type atoms is retrieved by minimizing the information loss during the formation of the molecules. The obtained results are promising and generalize previous models.

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COMPUTATIONAL CHEMISTRY STUDIES ON ATMOSPHERICALLY-RELEVANT ORGANIC COMPLEXES WITH IRON

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Computational studies of atmospheric aerosols is used in understanding the overall reactivity of these particles due to reactions with trace gases or those induced by absorbing solar radiation. Humic like substances in aerosols (HULIS) are considered an important class of macromolecules due to their unique photochemical properites and ability to complex to transition metals such as iron. Simple models for HULIS include gallic acid (GA) and catechol (PC). Our goal is construct clusters that mimic the ones in real aerosol systems and completely characterize the structural, electronic and vibrational properties for comparison with similar data collected experimentally. We use Density Functional Theory and the B3LYP/6-31G(d) method and basis set to analyze the changes that occur in the electronic spectra of GA and PC as they interact with iron. We used Spartan, Gaussian and ChemCraft to run the calculations. To simulate water on the surface of aerosols that faciliate ionic mobilty, explicit and implicit solvation was taken into account in our calcualtions. We looked at the effect of solvation on geometrical parameters, electronic and infrared spectra. Results obtained from calculations were then compared with experimental data collected using x-ray diffraction, UV-vis and infrared spectroscopies. The implication of our results on modeling heterogeneous photochemical reactivity of these clusters will be discussed.

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Toward approximating the exchange-correlation potential by explicit modeling of the exchange-correlation charge distribution

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The problem of approximating the exchange-correlation potential in potential-driven density-functional theory can be viewed from the perspective of electrostatics. In this case, the potential $v_{\rm XC}(\mathbf{r})$ can be modeled indirectly in the form of the associated exchange-correlation charge distribution $q_{\rm XC}(\mathbf{r})$. This implies working in terms of known constraints, which are to be imposed on the function $q_{\rm XC}(\mathbf{r})$. As an example of such a constraint, we devise analytic integrability conditions that a model $q_{\rm XC}(\mathbf{r})$ must satisfy in order for the resulting potential to be a functional derivative. We also discuss the use of another important property of $q_{\rm XC}(\mathbf{r})$, the normalization constraint, which is responsible for the correct asymptotic behavior of the corresponding $v_{\rm XC}(\mathbf{r})$.

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Variational Principles in Wave-Functional and Density-Functional Formulations of Quantum Mechanics

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Variational theorems are important for obtaining approximate solutions to the Schroedinger equation. With this in mind, fundamental variational principles will first be discussed within the wave-functional formulation of quantum mechanics. Then the corresponding variational principles for ground states in density and density-matrix functional theories will be reviewed briefly for the non-degenerate and degenerate situations. Based on these variational principles, properties of the exact functionals will be presented that are difficult to satisfy with approximate functionals. Special emphasis will be given to degeneracies, coordinate scaling, and potentials (functional derivatives). Then, a new time-independent density-functional theory for excited states will be presented for Coulomb systems. The lecture will conclude with a description of certain relevant unsolved mathematical problems, such as one involving an ionization energy convexity property.

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Accurate Bond Dissociation Curves at Mean-Field Computational Cost: Describing Strongly Correlated Systems with Nonorthogonal Geminals

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Antisymmetrized product of electron pairs (geminals) have been recognized as conceptually interesting and highly accurate wavefunctions since the early days of quantum chemistry.[1] In contrast to the conventional orbital approach, geminals make explicit use of the two-particle nature of the Hamiltonian. It was shown in the past that such geminal methods are a particular kind of one-electron reduced density matrix functionals.[2] Although very appealing from a fundamental point of view, until recently there were no computationally tractable approaches that did not impose severe restrictions on the geminals (*e.g.* strong orthogonality).[3] The computational cost without these approximations would be factorial (in fact $n!$ terms, each containing an n-by-n permanent, have to be evaluated) in the naïve approach. However, we propose alternative ways of parametrizing such permanents for a fast evaluation, and at the same time apply a projection scheme to reduce the overall computational cost to n^4.[4]

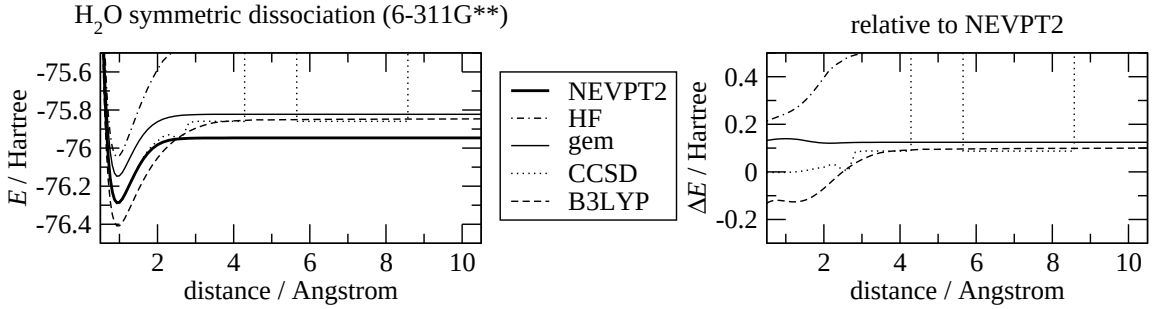

Figure 1: The symmetric H_2 removal from a water molecule is one of the hard problems for DFT (and even coupled-cluster running into some convergence problems at long distances) for which our method predicts values highly parallel to accurate calculations (NEVPT2)

We could show that this method is highly reliable for bond dissociations (Figure 1) and accurately models all effects of strong electron correlation, yet is computationally very inexpensive.

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Kohn-Sham model for heavy atoms

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The Density Functional Theory (DFT) of Kohn and Sham has emerged as the most widely-used method of electronic structure calculation in both quantum chemistry, condensed matter physics and materials science.

We study the standard and extended Kohn-Sham models for quasi-relativistic N-electron Coulomb systems describing heavy atoms; that is, systems where the kinetic energy of the electrons is given by the quasi-relativistic operator

$$\sqrt{-\alpha^{-2}\Delta_{x_n}+\alpha^{-4}}-\alpha^{-2}.$$

For spin-unpolarized systems in the local density approximation, we prove existence of a ground state (or minimizer) provided that the total charge Z_{tot} of K nuclei is greater than $N-1$ and that Z_{tot} is smaller than a critical charge $Z_{\text{c}}=2\alpha^{-1}\pi^{-1}$. The proof is based on the concentration-compactness approach to locally compact variational problems involving nonlocal operators.

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A density functional theory of hydrogen transfer for short-chain alkane thiols on small cationic, anionic, and neutral gold clusters

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Alkane thiols are commonly used in aqueous solutions to stabilize gold clusters and prevent their aggregation. In this study density functional theory was used to calculate the geometries and vibrational frequencies of cationic, anionic, and neutral gold clusters (Au_n, $n = 1-4$), bonded to hydrogen sulfide, H_2S, methane thiol, CH_3SH, and ethane thiol, CH_3CH_2SH. For gold, a pseudopotential was used to incorporate the large relativistic effects. Thermochemical values were calculated for the transfer of a hydrogen atom from sulfur to the gold cluster for each of the complexes studied. Significantly different results were obtained for the cationic, anionic, and neutral short-chain alkane thiol-gold cluster complexes.

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Towards reliable modeling of excited states of actindes from (relativistic) time-dependent density functional theory

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The uranium dioxocation (UO_2^{2+}) and its isoelectronic counterparts NUN and NUO^+ are the essential building blocks of many uranium species. These linear triatomic molecules can be further coordinated in the equatorial plane by three to six ligands [1]. Unfortunately, the nature of the chemical binding of the equatorial ligands to the uranium metal center is not yet fully understood. For better understanding of this phenomena, it is necessary to investigate the electronic spectra of different uranium-containing complexes. However, theoretical modeling of the electronic transitions of such heavy elements remains a challenging task for currently available quantum chemical methods as correlation and relativistic effects have to be treated on an equal footing.

The aim of this work is to model the electronic spectra of small uranium complexes employing wave function methods such as Complete Active Space Second-Order Perturbation Theory (CASPT2) and Intermediate Hamiltonian Fock-Space Coupled Cluster (IHFSCC) and asses the accuracy of Time-Dependent Density Functional Theory (TD-DFT) [2, 3]. The performance of different exchange–correlation functionals is tested for the spin-free and spin–orbit coupling vertical excitation energies. In addition, the importance of the Gaunt interaction in the TD-DFT spectra is discussed.

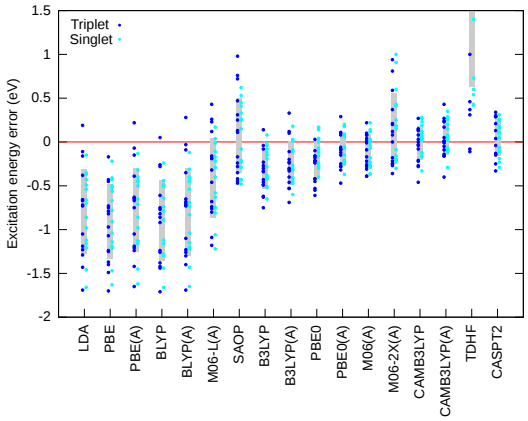

Figure 1: Performance of different exchange–correlation functionals for the spin–free vertical excitation energies with respect to IHFSCC.

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A new DFT approach to polarizable force-fields

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Sanderson's principle of electronegativity equalization states that, upon formation of a molecule, electrons flow until all electronegativities are equalized. Essentially the same principle is found in density functional theory (DFT), stating that the electronic ground state has a constant chemical potential. Starting from basic DFT equations, Mortier et al. derived the electronegativity equalization method (EEM), providing an elegant mathematical reformulation of Sanderson's principle [1]. The molecular electronic energy is approximated to second order in terms of atomic charges. Minimization of this energy with a total charge constraint leads to a set of linear electronegativity equations, predicting fairly accurate atomic partial charges. In principle, EEM could also be used to describe electronic linear response properties such as the molecular dipole polarizability or the dielectric constant of a crystal.

A polarizable force-field is essentially a generalization of the EEM, often including inducible atomic dipoles (and quadrupoles). It is even very common to fix the atomic charges and to describe the linear response properties with only the inducible dipoles. At first sight, it is counter-intuitive to neglect the response contributions from the atomic monopoles and to work only with the contributions from higher multipoles. However, this tendency in the literature can be explained on the basis of the fundamental limitations of EEM, which were only revealed recently. The EEM predicts that the dipole polarizability of a chain molecule grows cubically with the chain length, while one expects a linear trend in the macroscopic limit for dielectric molecules [2]. Furthermore, EEM predicts a non-integer charge transfer between different molecules, even when they are well separated. These problems limit the applicability of the EEM to small isolated molecules where an incorrect polarizability is acceptable.

In this talk, we propose a successor for the EEM: "Atom-Condensed Kohn-Sham DFT approximated to second order" (ACKS2) [3]. Relying on principles from constrained DFT and the Legendre transform of the Kohn-Sham kinetic energy, a more general approximation for the electronic energy in terms of atomic populations is derived from Kohn-Sham DFT. This new form can exhibit both metallic and dielectric limits for the dipole polarizability (in analogy with the split-charge equilibration [4]) and enables a correct dissociation limit for the atomic partial charges. A minimization of the ACKS2 energy with a total charge constraint leads to a set of linear equations that only have a marginal computational overhead compared to the EEM equations. Computational benchmarks of the ACKS2 model show that the good prediction of the anisotropy of the dipole polarizability is one of the particular strengths of the model.

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Decisions and Games (SS-DG)

Organizers:
D. Marc Kilgour (Wilfrid Laurier University)
Marcus Pivato (Trent University)

Which course of action is best? What is a decision-maker's rational choice? For deterministic problems with a clear objective, this question can be answered using optimization. In a setting of uncertainty, however, is the province of the subjective expected utility theory of Ramsey, de Finetti, and Savage, which has been extended to deal with ambiguity, multiple objectives, multiple attributes, and intertemporal decisions. But strategic uncertainty, resulting from the presence of other decision-makers with their own options and objectives, was recognized by von Neumann and Morgenstern to require new methods. Game theory, their system to model strategic interaction, was augmented by contributions from Nash, Harsanyi, Aumann, and many others, and has now revolutionized economics and made substantial impacts in political science and other social sciences. This session will feature new applications of mathematics that are inspired by attempts to understand decisions and games.

Social Choice Theory (SS-SCT)

Organizers:
D. Marc Kilgour (Wilfrid Laurier University)
Marcus Pivato (Trent University)

How should a group of people make a collective decision? Elect a government? Divide a common resource? Match claimants to indivisible resources? Aggregate individual judgements into a logically consistent consensus? Combine private information in an epistemically optimal way? Negotiate an agreement? Many rules have been proposed to produce collective decisions, but their appropriateness has been debated. Is the implementation of a rule computationally complex? Is the rule susceptible to manipulation, and if so how complex is that manipulation? Is the rule vulnerable to paradox and inconsistency? If a rule is internally consistent, socially efficient, and procedurally fair, is that enough? Or should it instantiate some theory of social justice? Can the conflicting norms of welfare, fairness, and collective rationality ever be reconciled? These are some of the questions that the mathematical theory of social choice seeks to answer.

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Analogy in Decision-Making

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In the context of decision making under uncertainty, I formalize the concept of analogy: an *Analogy* between two decision problems is a mapping that transforms one problem into the other while preserving the problem's structure. After identifying the basic strcture of a decision problem, I introduce the concepts of *Analogical Reasoning Operator* and of *Analogical Reasoning Preference*. The former maps the decision problem at hand into a family of decision problems, which are analogous to the problem under consideration. The latter is the result of aggregating the various analogies. I provide several representations (in decreasing order of generality) of the analogical reasoning operators. After introducing two mild assumptions on the aggregators of analogies, I characterize analogical reasoning (AR) preferences. I give several examples of AR preferences and of the associated aggregators. These include Gilboa-Schmeidler similarities, Choquet integrals and quantiles. Finally, I show that the class of Monotone Continuous Invariant Bi-separable (MCIB) preferences (which includes many popular models of decision making under uncertainty) has an important stability property: Any MCIB preference is an AR preference; conversely, every AR preference which results from aggregating MCIB preferences is an MCIB preference.

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Fast Equilibrium Computation for Infinitely Repeated Games

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It is known that an equilibrium of an infinitely repeated two-player game (with limit average payoffs) can be computed in polynomial time, as follows: according to the folk theorem, we compute minimax strategies for both players to calculate the punishment values, and subsequently find a mixture over outcomes that exceeds these punishment values. However, for very large games, even computing minimax strategies can be prohibitive. In this paper, we propose an algorithmic framework for computing equilibria of repeated games that does not require linear programming and that does not necessarily need to inspect all payoffs of the game. This algorithm necessarily sometimes fails to compute an equilibrium, but we mathematically demonstrate that most of the time it succeeds quickly on uniformly random games, and experimentally demonstrate this for other classes of games. This also holds for games with more than two players, for which no efficient general algorithms are known.

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Fair Division

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Over the past 20 years, there has been burgeoning interest in the subject of fair division—how one divides a single divisible good (e.g., a cake), or multiple indivisible goods (e.g., the marital property in a divorce), that satisfy such properties as efficiency, envy-freeness, and equitability. Some of the major possibility and impossibility results—relating to both the existence of such a division and algorithms for producing it—will be reviewed. How these results apply to dividing land, allocating items in a family estate to heirs, determining which rooms housemates get and how much of the rent each pays for its room, and matching applicants to colleges will be among the applications discussed.

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On the existence of Berge equilibrium with pseudocontinuous payoffs

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The concept of Berge equilibrium goes back to the book of Berge (1957) and was later formalized by Zhukovskii (1994) for differential games. For a non cooperative game with finite number of persons, this equilibrium means that if each person plays his strategy at a Berge equilibrium, then he obtains the maximum payoff if all the remaining players play their strategy in the Berge equilibrium. It is worthnoticing that the Berge equilibrium is totally different from the Nash equilibrium since the Nash equilibrium is stable with respect the deviation of any unique player. For the concept of Nash equilibrium, we refer the reader to the paper of Nash (1951). The existence of Berge equilibrium has been studied by Nessah et al (2007), Larbani and Nessah (2008), Abalo and Kostreva (2004, 2005) and Colman et al (2011). More recently, Musy et al (2012) have established the existence of Berge equilibrium without using Nash equilibrium. Previously mentioned works, the authors have assumed that payoffs of persons are continuous. However, many games as the oligopolies of Bertrand (1883) and Hotelling (1929) have discontinuous payoffs. Several authors have studied the existence of Nash equilibrium where payoffs are not necessarily continuous. Let us quote for example, Morgan and Scalso (2007). In their paper, Morgan and Scalso (2007) have proved the existence of Nash equilibrium with ‘‘pseudocontinuous’’ payoffs. In this work we prove the existence of Berge equilibrium with ‘‘pseudocontinuous’’ payoffs.

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The variable choice set logit model applied to the 2004 Canadian election

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Formal work on the electoral model often suggests that parties should locate at the electoral mean. Recent research has found no evidence of such convergence. In order to explain non-convergence, the stochastic electoral model is extended by including a competence and sociodemographic valance in a country where regional and national parties compete in the election. That is, the model allows voters to face different sets of parties in different regions. We introduce the notion of a convergence coefficient, c for regional and national parties and show that when c is high there is a significant centrifugal tendency acting on parties. An electoral survey of the 2004 election in Canada is used to construct a stochastic electoral model of the election with two regions: Québec and the rest of Canada. The survey allows us to estimate voter positions in the policy space. The variable choice set logit model is used to built a relationship between party position and vote share. We find that in the local Nash equilibrium for the election the two main parties with high competence valence, the Liberals and Conservatives, locate at the national electoral mean and the Bloc Québécois, with the highest competence valence, locates at the Québec electoral mean. The New Democratic Party has a low competence valence but remains at the national mean. The Greens, with lowest competence valence, locate away from the national mean to increase its vote share.

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Degree of Difficulty: A Fundamental Problem of Contest Design

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Rewards received by economic agents are typically cardinal measures of performance, but sometimes they are, at least in part, ordinal. It is well-established that rewards—cardinal or ordinal—can rationally motivate increased effort. We ask whether the cardinal or ordinal nature of the reward can affect contestants' strategies. Specifically, if level of effort is fixed and level of difficulty is the only choice, what strategy is optimal? For example, in a high-jump competition, level of effort can be considered fixed, and the only strategic choice is height attempted, or level of difficulty. Assuming that only successful candidates, or only more successful candidates, are rewarded, and that the reward may depend on level of difficulty, we study whether and how the nature of the reward

can affect optimal strategies. Basing our conclusions in part on simple probabilistic models where optimal choices can be determined analytically, we show that the structure of competitive rewards can alter contestants' rational choices. We adopt a contest-design framework: What combinations

of fixed and variable prizes cause contestants to select levels of difficulty that maximize the contest designer's expected payoff? Our general conclusion is that competition can affect strategic choices, in magnitudes and even directions that are difficult to predict.

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Comparing Mutually Naïve and Strategic Sequential Selection

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Consider two players who divide n indivisible items by alternating selection of one item at a time. The players may value the items in different orders. Requiring each player to have a strict ranking over the n items, their relative preferences can be encoded in a permutation on n letters, allowing tools of algebraic combinatorics to be used in analysis of this situation [3, 2].

When neither player knows the other's ranking of the items, each simply chooses her favorite item still available when it is her turn, the naïve strategy. When there is "one-way" knowledge, the player with knowledge predictably does better on average than the player using the naïve strategy. When both players have knowledge of the opponent's preferences, the optimal selection strategy is known [4], essentially working backwards from the last move, leading to the name "bottom-up" strategy [1].

For instance, labeling the items so that the first player's preference over six items is $1, 2, 3, 4, 5, 6$, suppose the second player's preference is $\pi = 2, 6, 3, 4, 5, 1$. Optimal play in the four possible states of knowledge is summarized in the following table (where outcomes for the second player are also presented in terms of her preferences).

	2nd naïve	2nd strategic
1st naïve	$\{1,3,4\},\{2,5,6\} = \{\pi(1),\pi(2),\pi(5)\}$	$\{1,3,5\},\{2,4,6\} = \{\pi(1),\pi(2),\pi(4)\}$
1st strategic	$\{1,2,3\},\{4,5,6\} = \{\pi(2),\pi(4),\pi(5)\}$	$\{1,2,4\},\{3,5,6\} = \{\pi(2),\pi(3),\pi(5)\}$

Notice that, in this example, among the two possibilities where players have the same level of knowledge, the first player does better in the mutually strategic situation (1st, 2nd, and 4th ranked items versus 1st, 3rd, and 4th), while the second player does better in the mutually naïve situation (1st, 2nd, and 5th versus 2nd, 3rd, and 5th). Is this always the case?

The current work shows that, on average, both players fare equally well under mutually naïve and mutually strategic play. Moreover, this is true no matter "how different" the players' preferences are. More specifically, the distance between permutations can be measured by the minimal number of pairs of neighborly transpositions (of the form $(i, i+1)$) necessary to go from one to the other. The stronger result shows that, for any fixed permutation distance, both players fare equally well under mutually naïve and mutually strategic play among preferences that differ by that distance.

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Enumeration and Connections for Extensive-Form Games

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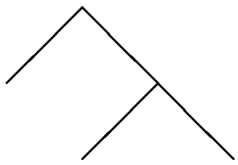
A foundation of game theory, 2×2 normal-form games with strict ordinal preferences have been widely studied [3]. Enumeration was extended to 2×2 games where ties are allowed in 1986 [1]. Recently, a system of connecting strict ordinal preference 2×2 games has been developed [4] and extended to games with ties [2].

Another important game theory model is the extensive-form game. This model, often represented as a tree, allows more freedom to accommodate multiple players and varying numbers of options in the course of sequential moves. Even restricting to ordinal preferences, the number of possible extensive-form games grows rapidly with the number of possible outcomes.

The current work considers extensive-form games for two players having ordinal preferences over small numbers of outcomes. Enumeration results are derived for both strict and non-strict ordinal preferences. Further, the Robinson-Goforth system of connecting games [4] is extended to this setting, providing for a meaningful notion of distance between games and a helpful context for considering all possible games based on the same tree graph.

For example, there are 18 games using the tree shown below where both players have strict preferences over the three outcomes. Connecting these games into a 4-regular graph, using swaps of adjacent preferences as edges, shows that the games partition into three classes with a maximum distance of 5 between any two games. Embedding the 18-vertex structure into a richer setting in the style of [2] allows for the inclusion of games with ties.



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Implementation of Majority Voting Rules

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In this paper, I study implementation by agenda voting, a straightforward mechanism that is widely used in practice. The main result establishes that any candidate neutral majority voting rule which satisfies the two necessary conditions identified in prior work (McKelvey and Niemi [1]; Moulin [2]) as well as a significantly weakened version of Sen's α [3] can be implemented by sophisticated voting on an agenda.

The sufficient conditions are satisfied by almost every majority voting rule discussed in the literature, including the *Uncovered Set*, the *Banks Set*, the *Minimal Covering Set*, the *Bipartisan Set*, the *Tournament Equilibrium Set*, and the *Slater Set*. This effectively shows that the *Copeland Set* is the only popular majority voting rule which is not agenda implementable. Having said this, the Copeland Set can be implemented "approximately" in the sense that there exists an agenda such that the Copeland score of any sophisticated voting outcome is at least two-thirds that of the Copeland winner(s).

The main result also clarifies what can be implemented via dominance solvable voting and backward induction, two appealing yet poorly understood solution concepts related to agenda voting.

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When Does Approval Voting Make the "Right Choices"?

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We assume that a voter's approval of a proposal depends on (i) the proposal's probability of being right (or good or just) and (ii) the voter's probability of making a correct judgment about its rightness (or wrongness). The state of a proposal (right or wrong), and the correctness of a voter's judgment about it, are assumed, initially, to be independent. If the average probability that voters are correct in their judgments is greater than ½, then the proposal with the greatest probability of being right will, in expectation, receive the greatest number of approval votes. This result also holds when voters' probabilities of being correct are state dependent but not proposal dependent; when they are functionally related in a certain way; or when voters follow a leader with an above-average probability of correctly judging proposals. Sometimes, however, voters will more frequently select the right proposal by not following a leader and, instead, making their own independent judgments (as assumed by the Condorcet jury theorem). Applications of these results to different kinds of voting situations are discussed.

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The relationship between Arrowian social welfare function and the distance-based inconsistencies in pairwise comparisons

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Pairwise comparisons (PC) must have been used before numbers have been invented and modern mathematics established. It is the most natural way of comparing two objects. Ramon Llull was given credit for discovering the Borda count and Condorcet criterion (Llull winner) in the 13th century but the true theoretical foundations have been established by Thurstone in 1927 as the "law of comparative judgment". Interestingly enough, when additional PC input is considered, Arrowian social welfare function can be constructed. However, the researchof the most important concepts in PC is still ongoing. A distance-based inconsistency defined in 1993 in [2] as a minimal distance from the nearest consistent triad in PC matrix A. The distance-based inconsistency localizes the most inconsistent triad (or triads). It is the maximum over all triads a_{ik}, a_{kj}, a_{ij} of elements of A (say, with all indices i,j,k distinct) of their inconsistency indicators, which can be defined as:

$$ii = 1 - \min\left(\frac{a_{ij}}{a_{ik}a_{kj}}, \frac{a_{ik}a_{kj}}{a_{ij}}\right). \quad (1)$$

In [1] a proof of convergence has been provided for the distance-based inconsistency. However, it was a mathematical (existential) proof. No empirical study has been ever done and this is the first publication showing how fast convergence takes place. In our experimentation, we modify all three values: a_{ik}, a_{kj}, and a_{ij}. It is done by splitting the total modification to three elements of a triad according to their relative weights. The weight-based inconsistency reduction algorithm can efficiently reduce the global inconsistency of a PC matrix under a certain threshold value (1/3 is considered as the acceptable inconsistent level). We can control the deviation in generated inconsistent PC matrices for our experimentation in the following way. The NSI PC matrix A is obtained from a random vector v by $A = [v_i/v_j]$. A random deviation is applied on all the elements in the upper triangle to make matrix A inconsistent. In order to test the convergence of weight-based method of inconsistency reduction, we:
- generate 1,000 random not-so-inconsistent (NSI) PC matrices according to the method described above,
- add a deviation of 0.5 on each entry in the upper triangle,
- finding the maximal inconsistency of each PC matrix,
- counting the number of iterations needed to reduce the maximal inconsistency of the PC matrix to not more than 1/3. The result shows that the convergence was fast and rather surprising. Bringing matrices to inconsistency bellow 1/3 takes place usually in not more than 10 steps.

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Selfish driving behaviour and its effects on highway traffic

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We model deviations from the norm behaviour of drivers, taking place on a stretch of highway traffic. The norm behaviour is described by drivers respecting the laws and rules of traffic; the deviant behaviour (or defecting from the norm) is defined as drivers who enlarge their set of strategies by strategies outside of the laws and rules of traffic (such as passing on the right, tailgating, merging too soon, etc.). Each driver has an innate probability of acting selfish, and in certain traffic conditions a driver can choose among a finite set of deviant strategies. We are studying the effect selfish driving has on the overall traffic conditions (such as appearance of congestion). The long term value of this research is be show that traffic flow and efficiency (defined as minimizing time on the road for each driver) can be increased though improving drivers' behaviour.

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Ranking Multidimensional Alternatives and Uncertain Prospects

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We introduce a two-stage ranking of multidimensional alternatives, including uncertain prospects as particular case, when these objects can be given a suitable matrix form. The first stage defines a ranking of rows and a ranking of columns, and the second stage ranks matrices by applying natural monotonicity conditions to these auxiliary rankings. Owing to the Debreu-Gorman theory of additive separability, this framework is sufficient to generate very precise numerical representations. We apply them to three main types of multidimensional objects: streams of commodity baskets through time, monetary input-output matrices, and most extensively, uncertain prospects either in a social or an individual context of decision. Among other applications, the new approach delivers the strongest existing form of Harsanyi's (1955) Aggregation Theorem and casts light on the classic comparison between the *ex ante* and *ex post* Pareto principle. It also provides a novel derivation of subjective probability from preferences, in the style of Anscombe and Aumann (1963).

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Condorcet VS Borda, round $n+1$

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We know from the Gibbard-Satterthwaite Theorem that with three or more alternatives every resolute, non-imposing, and non-dictatorial social choice function (SCF) is manipulable. We prove a variant of this theorem that uses stronger hypotheses and provides additional information, revealing a fundamental dichotomy in the *type* of strategic vulnerability for an SCF.

Theorem 1 *(Stated loosely)* With four or more alternatives every resolute, neutral, and anonymous SCF f is either:

- Free from the reversal paradox, but manipulable on the subdomain $\mathscr{D}_{Condorcet}$, or
- Strategy-proof on $\mathscr{D}_{Condorcet}$ but suffers from the *reversal paradox* for some profile $P \notin \mathscr{D}_{Condorcet}$, *or*
- Suffers from both problems.

Terminology A *resolute SCF* is a voting rule that returns a unique winning alternative (no ties allowed) for each profile of strict (linear) preferences over a finite set A of alternatives (aka "candidates").

In a *reversal paradox* a voter changes the winner to one she strictly prefers by completely reversing her sincere ranking. A reversal represents a maximally insincere ballot – for every pair of alternatives, it misstates which of the two the voter prefers – and so a reversal paradox represents a particularly extreme form of manipulability.

A *Condorcet alternative* x is preferred to each other alternative y by a strict majority of voters, and $\mathscr{D}_{Condorcet}$ is the subdomain consisting of all profiles for which a Condorcet alternative exists. *Pairwise Majority Rule* selects the *Condorcet alternative* for each profile in $\mathscr{D}_{Condorcet}$. A *Condorcet extension* is an SCF that agrees with PMR on $\mathscr{D}_{Condorcet}$.

Comment The precise statement of Theorem 1 relaxes the neutrality and anonymity hypotheses but requires a minimum number of voters (which is increasing in the number of alternatives). The proof combines two earlier results. Campbell and Kelly [1] show that Condorcet extensions are the *only* strategy-proof SCFs on $\mathscr{D}_{Condorcet}$ (assuming weak forms of neutrality and anonymity), while Sanver and Zwicker [2] show that resolute Condorcet extensions for four or more alternatives suffer from the reversal paradox. The latter result is a strong form of Moulin's theorem in [3], [4] that resolute Condorcet extensions suffer from the *no-show paradox*.

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Evolutionary Game Theory (SS-EGT)

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

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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Infinite Niche Packing

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The evolutionary games literature has extensive coverage on the coexistence of finite number of strategies with very little discussion on the possibility of coexistence of infinite number of strategies. Gyllenberg and Meszéna ([1]) give an example of an infinite niche packing and note that such examples are not robust. Specifically, they show under some conditions that there is always a slight perturbation of the intrinsic growth rate such that the perturbed model has no equilibrium with support having a limit point. However, these results leave open the possibility that other slight perturbations maintain an equilibrium with continuous support. Our interest is in the latter possibility and we examine it with a one-dimensional model for the evolution of strategy frequencies based on the fitness function

$$\pi(x,y) = 1 - e^{-(x-y)^2/(2\sigma^2)} \frac{e^{-y^2/2}}{e^{-x^2/2}}. \tag{1}$$

When $\sigma^2 > 1$, this model has one monomorphic strategy that is an ESS and NIS, and thus is convergence stable. When $\sigma^2 < 1$, the monomorphic strategy is no longer an ESS but is a NIS with the implication that multiple (finite or infinite) strategies may be present in an equilibrium. Results from numerical simulations of the Darwinian dynamics ([2]) for the above model when $\sigma^2 < 1$ will be discussed.

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Game-theoretic methods for functional response and optimal foraging behavior

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The number of prey of a given type consumed by a predator per unit time (i.e. the functional response) depends on the spatial distribution of the prey as well as on the decisions taken by the predator (e.g. where to search for prey, which type of prey to pursue, whether to attack, etc.) and on the times taken for these activities relative to their expected nutritional value gained. I will discuss (i) how this information can be conveniently represented in a tree diagram similar to an extensive form game; (ii) how standard functional responses such as Holling II emerge naturally from this setting; (iii) how game-theoretic methods can be used to analyze the optimal foraging strategy of the predator. The methods will be illustrated for classical diet choice and patch choice models, including those that involve the effects of simultaneously encountering different types of prey and of prey recognition effects. They will also be applied to predict equilibrium foraging behavior of a predator population with intraspecific strategies taken from a Hawk-Dove game that includes interaction times.

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Plants and games: adaptive strategies for nutrient foraging and competition

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Plants experience an ever changing environment, and are adept at assessing and responding to external cues. For example, nutrients are often patchily distributed in soil, and the majority of plants will place more roots inside nutrient rich patches compared to nutrient poor patches. Similarly, competition among plants belowground is fierce, and some plants respond to neighbours by increasing root production. Here, a game theoretical framework for adaptive root production, and its ecological consequences is presented.

Let the total nutrient harvest by plants, $H_i(v,u)$, increase with root production (u_{ij}), nutrient encounter rate (a_{ij}) and the abundance of resource i (R_i), but with diminishing returns given by,

$$H_i(v,u) = R_i\left(1 - e^{\sum a_{ij}u_j}\right).$$

It is assumed that competing plants divide up the total nutrient harvest $H_i(v,u)$, proportional to their contribution to the total uptake capacity of the community, and that root costs, c_k, scale linearly with root production. Thus net fitness, $G_k(v,u)$, of plant k, foraging on n substitutable resources, is given by,

$$G_k(v,u) = \sum_{i=1}^{n} \frac{a_{ik}u_k}{\sum_{j=1}^{k} a_{ij}u_j} H_i(v,u) - c_k u_k \ .$$

For a plant foraging for nutrients in the absence of competition (*i.e.* $a_{ik}u_k = \Sigma a_{ij}u_j$) the optimal root production is given by $u_k^* = \ln(a_{ik}R_i/c_k)/a_{ik}$. For plants foraging with neighbours, u_k^* must be found numerically. When $a_{ik}=a_{ij}$ and $c_k=c_j$ the game is symmetric and captures intraspecific competition. When $a_{ik}\neq a_{ij}$ and $c_k\neq c_j$ the game is asymmetric and captures interspecific competition.

Figure 1 shows the basic relationship between parameters and ESS root production. Generally, the model predicts that intraspecific competition is more intense than interspecific competition leading to higher ESS root production. Introducing multiple resources into the game allows for resource partitioning which eases competition, and therefore lowers ESS root production. Some implications of these game-theoretic plant foraging strategies for plant community ecology will be discussed.

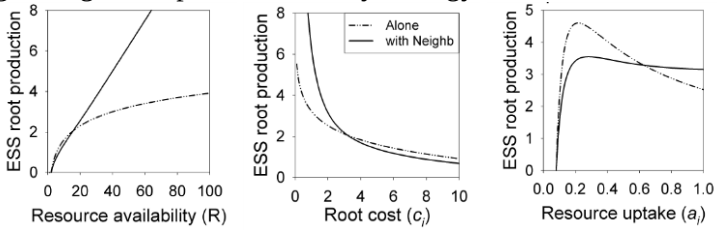

Figure 1: ESS root production relative to resources (left), root costs (centre), and uptake capacity (right).

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Dynamics of pattern networks in rock-paper-scissors type models

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We consider rock-paper-scissors type models with an arbitrary number of species and study realizations which lead to the formation of domains composed a single species. These domains are bounded by interfaces of empty sites generated by predation of identical strength between competing species. We have shown that while models with a symmetric bidirectional predation interaction between all species lead to interface networks with multiple junctions (left panels of Fig. 1), models with one N-cyclic predator-prey rule may lead to a population network with N-armed spiral patterns (right panel of Fig. 1). We investigate the dynamics of interface networks and show that they evolve obeying the scaling law $L \propto t^{1/2}$, where L is the characteristic length of the network and t is the time. In contrast, the spiral pattern networks are not curvature driven and have a nearly constant characteristic length scale at late times as it was shown in Ref. [1]. We demonstrate in Ref. [2] that the interface networks are similar to those of several other nonlinear systems.

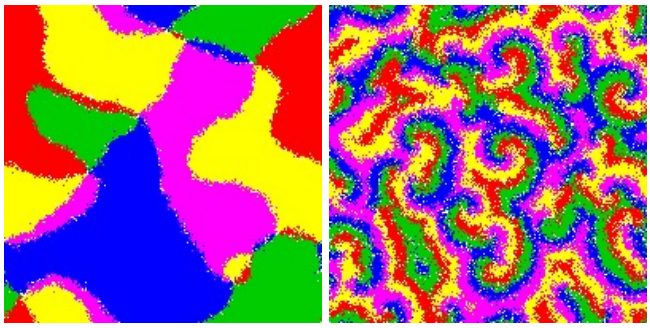

Figure 1: Snapshots of numerical simulations of the rock-paper-scissors model with 5 species. Depending on the predation probabilities between the species, interface networks with junctions and spiral patterns are formed.

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Habitat Selection for the Ideal Free Distribution in Linear and Nonlinear (Allee Effect) Fitness

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We look at Fretwell and Lucas' (1969) article On Territorial Behaviour and Other Factors Influencing Habitat Distribution in Birds, to provide further explanation for the relationships between bird dispersal over available habitats and their habitat distribution. Fretwell and Lucas (1969) introduced the Ideal Free Distribution (IFD) to predict how birds establish themselves among habitats. An IFD is a way in which animals distribute themselves among several resource patches. The number of individuals that will migrate among various patches is proportional to the amount of resources available in each habitat, whereby the distribution of individuals (birds) among patches will minimize resource competition and maximize fitness.
It has been shown that the IFD is an evolutionarily stable strategy (ESS) of the habitat selection game when fitness is a decreasing function of patch density. An ESS is a Nash Equilibrium (NE) strategy which, if adopted by a population of players, cannot be invaded by any alternative (mutant) strategy under the influence of natural selection. The influence of some of these factors is density dependent so that the suitability in a habitat is affected by the density of birds. Fretwell and Lucas assumed initially that the effect of density is always a decrease in suitability with an increase in density, which is contrary to the Allee principle. Allee's principle states that survival and reproduction rates increase when population size is small until it reaches some threshold value K, then rates decrease once this size is larger than K.
We develop a formula for the IFD when fitness functions are linearly decreasing and when their functions increase with population size until some maximum threshold is reached. We will extend the NE, ESS, and habitat selection game concepts to the case of the Allee effect.

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Interspecific Strategic Effects of Mobility in Predator-prey Systems

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In this talk, we will 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 chaotic behavior. Our investigation reveals the relationship between the game theory-based reactions of prey and predators, and their population changes.

Geocomputational Landscapes and Spaces (SS-GLS)

Organizers:
Steven A. Roberts (Wilfrid Laurier University)
Colin Robertson (Wilfrid Laurier University)

In this session we bring together researchers whose work in Geography and Environmental Studies relies on the extensive use or development of new geocomputational tools. More specifically, we explore computational solutions to problems related to the configuration of features in the landscape. These methodologies often involve concern with configuration of the solutions in the mathematical spaces of their expression. For example, there will be two papers presented on the solution of multiobjective optimization problems (in 7 or greater objectives) in a combinatorial setting (greenlands system design) with a focus on the tractable computing and analysis of estimates of Pareto optimal solutions. Further papers present findings on model checking using metrics for map comparisons. Additional presentations on related topics will fill out the session.

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Reducing Objectives in Many-Objective Optimization Problems for Landscape Design

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Most of the optimization problems in engineering have multiple objectives that must be optimized at the same time. They are named multi-objective optimization problems. The solution for these algorithms is composed by a set of solutions (instead of only one single solution) called the Pareto front. The algorithms to solve them grow exponentially their complexity when the number of objectives increases. Actually, the most popular multiobjective Evolutionary Algorithms (such as NSGA-II, PISA, etc.) have difficulties approximating the optimal Pareto front when the number of objectives is greater than 3 (called many-objective problems). The hypervolume-based algorithms have demonstrated to be capable to find good solutions for many objective problems, however they requiere large execution time. A very recent algorithm Partition and Selection Algorithm (PSA) [3] proposes a simple mechanism to improve diversity mechanism in many-objective evolutionary algorithms. On the other hand, the reduction of objectives is a viable alternative to deal this problem. If the number of objectives is reduced without altering the solution (or until a certain acceptable error) the problem could be solved by the current well established algorithms, reducing the execution time and improving the approximation to the Pareto front. Additionally, the visualization/analisys of the final Pareto front is easier handled by the final Decision Maker.

In this research we study the reduction of objectives with a heuristic method incorporated to an evolutive multiobjective algorithm (PSA in this case). The goal is to reduce the execution time by evaluating only a subset of objective functions at each algorithm iteration without affecting its overall performance. In addition to that, some strategies are used to make more affordable the process of analyzing the final Pareto front, such as the usage of the relation called *favour* ([1]) to differentiate between non-dominated solutions. The strategies are tested on some benchmark sets, also in a case of study referent to a combinatorial many-objective problem to landscape design [2]. This problem is conformed by eight objective functions refering to ecological configuration of lands. The goal is to decide what is the more convenient configuration for some portions of lands (considered as sites candidates to change) under the defined objective functions. This problem becomes hard to solve if the number of cadidate sites is large.

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LSP-GIS Method for Urban Land Suitability Decision-Making

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The Logic Scoring of Preference (LSP) method is a part of general multicriteria decision making approach that has origins in the soft computing [1]. The approach features an efficient nonlinear method for suitability aggregation and allows the expression of a spectrum of fuzzy logic requirements.

For more than two decades multicriteria analysis is used in geography in combination with geographic information systems (GIS) and for solving various spatial decision problems mostly related to land-use suitability [2]. However the commonly used weighting methods in the decision modeling procedures are based on weighted linear scoring (WLS) or analytical hierarchy process (AHP). They are driven by fixed (neutral) decision logic of factor compensation. However, nonlinear models of suitability, replaceability, and mandatory, sufficent, desired and optional requirements are important for real-world decision-making. The LSP method is offering all these nonlinear logic aggregators, based on the generalized conjunction/ disjunction (GCD) function with adjustable conjunction and disjunction degrees (andness and orness). Our implementation of GCD is based on weighted power means. The method can model simultaneity, replaceability, and a wide range of other aggregators to suit various evaluation objectives. Unlikely the WLS or AHP approaches, the LSP method is based on fuzzy reasoning and can aggregate an unlimited amount of inputs without loss of significance. However to date LSP method is mostly used in computer engineering and ecology, but its full potential in spatial and geographical applications is insufficiently explored [3, 4].

The main objective of this study is to develop and test an integrated method that incorporates LSP with GIS for the multicriteria decision-making of land suitability for new urban development. Geospatial data for Metro Vancouver Area, Canada, has been used to test the proposed method. Combining the requirements related to amenities (distance from coast and parks), accessibility (distance from roads and public transportation), population density (distance from residential housing and low density areas) and physical environment (elevation, slope, aspect) were used to build the aggregation structure of the model. Raster based GIS and IDRISI software has been used to implement the decision-making approach. The sensitivity analysis was performed to evaluate the performance of the number of inputs and logical requirements of the LSP-GIS methods. Obtained results indicate that LSP method is providing improved choices for multicriteria analysis of urban land suitability and thus has a potential for use in land-use planning and decision-making.

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Comparing Interpolation Techniques for Predicting Rainfall in Tropical Climates

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Environmentally–driven spatial models are increasingly require detailed, large–scale climatic datasets. In the context of rainfall mapping, spatial interpolation techniques are therefore requried to produce these inputs. While interpolation is straightforward for fully continuous phenomena like elevation and temperature, rainfall; as a semi-discrete process, is more challenging, as rainfall intensity interacts with both landscape and regional weather systems at a hierarchy of space-time scales. This is especially true in tropical settings. In this paper, four spatial interpolation techniques were analysed to test whether high quality precipitation data for Sri Lanka could be produced for use in future environmentally-driven models. The interpolation techniques tested were inverse distance weighting, thin plate smoothing splines, ordinary kriging, and Bayesian kriging.

Monthly precipitation data was interpolated for all of Sri Lanka from agricultural weather stations, and compared to both a network of official meteorological station readings, and satellite-based rainfall estimates. The objectives of the current research were threefold: investigate the potential for community managed weather stations to produce quality estimates of total monthly rainfall when compared to independent gold-standard meteorolgical station data, explore the use of a spatial analysis method for suplementing the assessment of interpolation pattern when compared to satellite-based rainfall measurements, and finally to produce seamless monthly rainfall maps for all of Sri Lanka. Absolute error, mean absolute error, median percentage error, standardized root-mean-square error, and the structural similarity index [1], an image comparison method, were used to assess which technique produced the best quality estimates. No particular interpolation method uniformly performed the best, but thin plate smoothing splines predicted the most accurately in high rainfall conditions, while Bayesian kriging performed the best with low rainfall. Establishing a threshold value for mean monthly rainfall under which Bayesian kriging will be used, and over which thin plate smoothing splines will be used was proposed as a solution.

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Evolutionary Multi-objective Optimization Design for Peri-urban Greenlands Systems: metric implementations

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Habitat fragmentation and loss, particularly in the urban fringe, is a key issue for land use planning and environmental policy implementation. Greenlands systems have been proposed as one solution to this issue [1]. This paper discusses aspects of the implementation of an Evolutionary Multi-objective Optimization (EMO) methodology for a greenlands system design [2]. The application of landscape ecology principles [3] via EMO combined with analysis of the Pareto front of non-dominated solutions and the measure of favour of these solutions provides a methodology to address the deterioration of ecological function in urban fringe areas and insights into the steps that can be taken to promote sustainable peri-urban landscapes.

This paper describes landscape design metrics from the implementation of an Evolutionary Multi-objective Optimization (EMO) algorithm for peri-urban greenlands system design. The results of particular landscape metrics using a real world data set of a small study area bring into relief issues concerning the interplay between the mathematization of landscape ecology principles of design and the resulting set of estimates of the Pareto optimal solutions. The paper discusses the research findings and provides links to other aspects of current EMO-based research methodology and its potential use as part of a landscape design decision support system. Specifically, this paper has two purposes. First, the design approach used may provide assistance to other researchers working to develop metrics and associated objective functions that incorporate landscape feature shape and configuration into decision support for environmental land-use planning. Second, the introduction of the new concept of anti-cut-set vertices, derived from the graph theoretic concept of cut-set vertices, allows some key connections to be identified between the larger sub-graphs in the dual graph of the study area's landscape features. This gives a very direct analytic tool for exploring potential conectivity structure in a given landscape.

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Map Comparisons and Model Checking: A Comparative Analysis

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Model assessment is an increasingly important aspect of spatial analysis. New sources of geographic information enable researchers to build complex spatial models. Additionally, Bayesian approaches to modelling are increasingly accessible to spatial researchers - either through simulation-based inference such as Markov chain monte carlo (MCMC) or advanced analytical techniques such as integrated nested Laplace approximations (INLA) - enable new ways to perform checks on model fit. When maps are the output of spatially explicit models, examining the spatial distribution of errors can improve understanding of mis-specification by suggesting missing covariates or identifying regional structures not present in the model. This paper explores techniques for assessing spatial structure of model residuals in the context of regular and irregular spatial lattices of a continuous mapped variable. The approach taken is analogous to continuous-value map comparison, however the focus of the paper is on spatial map comparison in the context of model assessment.

Given a map of a continuous variable Z which is indexed at all i locations across the study area, we obtain a second mapped continuous variable M, which is variable Z as represented in the model. Interest centres on comparing Z and M to assess the quality of predictions or as a goodness-of-it test. Typically, the mean of the squared errors (MSE) between Z and M is used as a criterion to evaluate prediction quality and/or model fit. Additional criterion employ penalties for the number of parameters used in the model (e.g., AIC, DIC). However, spatial patterning in the distribution of errors E is typically not considered.

In this study, a simulation experiment was developed to test the relative performance of various methods of spatial map comparison in the context of assessing structure of spatial model error. Gaussian Markov random fields were used to simulate Z, with various types of spatial dependence structures. For each Z, a M_i was generated by first transforming Z values and then resampling these values to new locations. Spatial resampling was developed to replicate various types of spatial structure errors including random allocation, scale, rotation, scale and rotation, and various gradients. For each M_i, MSE was determined, and each M_i were compared to the generating Z_i using the local and global versions of the Structural Similarity Index [1], global measures [2] of spatial autocorrelation (Moran's I and Geary's c) and local indicators [3] of spatial autocorrelation (local Moran's I and local Geary's c). The relative performance of each of the spatial analysis methods were compared using graphical and numerical summaries.

Spatial structure plays an important role in assessing the fit of complex spatially explicit models and understanding which methods are able to detect spatial structures in error under different error regimes can improve model development.

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Approximations to Intractable Spatial Econometric Models and Their Solutions Through Global Optimization

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Spatial econometrics, an interdisciplinary field involving applied mathematics, statistics, geography, and econometrics, focuses on incorporating spatial relationships into economic models. To understand the effects of these relationships, parameters of thse spatial models must be accurately estimated. As realistic models are thus far intractable, approximations are often made, but even in this case, the surrogate models have no analytic solution. This paper employs stochastic global optimization (specifically, particle swarm optimization (PSO) – a population-based iterative technique [1]) to estimate the parameters of the dynamic panel data model extended with a spatially lagged dependent variable [2]. Stochastic global optimization is an active research area, and shows great potential for estimating spatial econometric models [3].

Parameters of a simulated dynamic demand model for cigarettes are estimated from panel data (1963-1992) from 46 contiguous U.S. states [2]. The three-parameter autoregressive model is given as:

$$y_{i,t} = x_{i,t}\beta + \phi y_{i,t-1} + \kappa \mathbf{W} y_{i,t} + \varepsilon_{i,t} \quad (1)$$

where $x_{i,t}$ is the per capita disposable income, $\mathbf{W}$ is a binary contiguity matrix with $w_{i,j}$=1 if states i and j share a border, and $y_{i,0}$~$\mathbf{U}(0,4)$. For the simulation, the response variables $y_{i,t}$ are computed with β = -1.8, ϕ = 0.8, and κ = 0.5. The y for each state depend on the disposable income, the previous year's value of y in that state, and the current value of y in all other states that share a border with the state of interest.

Because there is no exact estimator of this model, two approximations: (1) Bhargava and Sargan (BS) and Nerlove an Balestra (NB) are employed [2]. For each approximation, three set of trials (total of 1000 iterations) using PSO were run, and the results averaged. The NB approximation returned values of β = -3.7031, κ = 0.3002 and ϕ = 1.1196. The BS approximation yielded the results β = -2.4516, κ = 0.1727 and ϕ = 1.3236 (see table below):

Approximation	Bias (κ)	Bias (ϕ)	Bias (β)	Fit with data (R^2)	Iterations
NB	-0.1998	0.3196	-1.9031	0.7205	1000
BS	-0.3273	0.5262	-0.6516	0.9597	1000

The results demonstrate that for intractable models, stochastic global optimization of approximations is viable in accurately estimating parameters in complex, non-convex search spaces. Additionally, data obtained during the optimization, such as population entropy and diversity, can be used to analyze search behaviour to further improve solutions, and to obtain analytic insight into stochastic search mechanisms.

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High-Order Methods in Computational Fluid Dynamics (SS-HOMCFD)

Organizers:
Lilia Krivodonova (University of Waterloo)
Hans De Sterck (University of Waterloo)

High-order methods provide an appealing approach for solution of complex problems in computational fluid dynamics. High-order methods are more efficient in terms of accuracy per degree of freedom or amount of computation. However, achieving the full potential of these schemes for nonlinear problems in complex geometries in the presence of shocks and other nonlinearities is challenging. This minisymposium will address recent developments in this area both from analytical and computational points of view.

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Accelerated High-Order Solver for the Cahn-Hilliard Equation on General Domains

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This research uses a recently introduced Fourier continuation method, the FC(Gram) [1, 2] method, to compute high-accuracy solutions to the Cahn-Hilliard equation [3] in three-dimensions. The FC(Gram) method enables use of the Fourier spectral method on non-periodic domains through efficient generation of a periodic continuation (Fig. 1a). An extension to the FC(Gram) method which enables the imposition of high-order Neumann boundary conditions is presented and validated. An open-source implementation of the FC(Gram) method with Neumann boundary conditions was developed which implements acceleration in fused CPU/GPU computing environments.

The FC(Gram)-Neumann method is found to have negligible affect on computational complexity of the algorithm, but reduces the effective order of spatial derivative approximation. Transient solutions to the Cahn-Hilliard equation of binary phase separation (Fig. 1b), a fourth-order partial differential equation, are shown to benefit from an approximate 10x speed-up on fused CPU/GPU architectures without loss of accuracy. Finally, an automated performance "tuning" method is presented and shown to enable optimal performance of the methodology in heterogeneous computing environments.

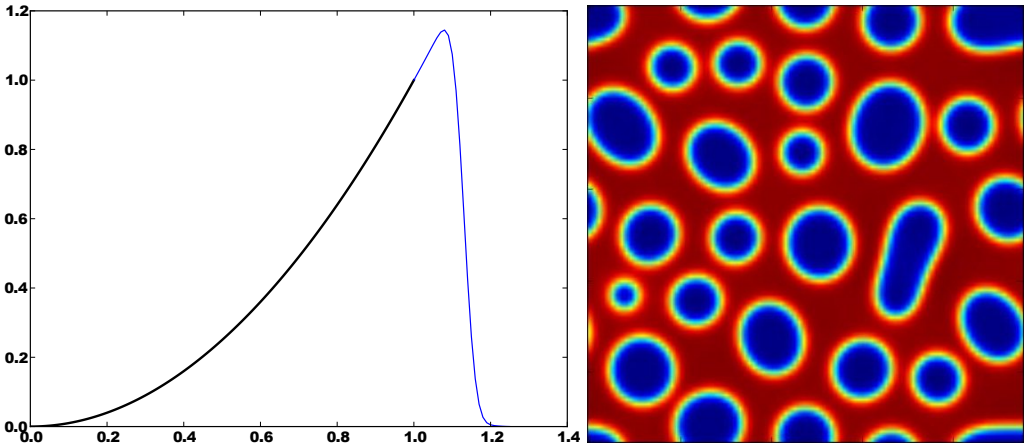

Figure 1: (left) Schematic demonstrating FC(Gram) method for the non-periodic function $f(x) = x^2$ (black) on the interval $[0,1]$ with periodic extension (blue); (right) Sample solution of the Cahn-Hilliard equation in two-dimensions.

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High-Order Finite Volume Element Methods for Elliptic PDEs with Singularities, and Applications to Capillarity

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Singular capillary surfaces in domains with sharp corners or cusps are well studied and the asymptotic series approximation of the solution is known. Yet it is also known that the singularity of the solution spoils the accuracy of standard finite element approximations, which cannot reproduce the singularity accurately. First we describe finite volume element methods for computing singular solutions of linear elliptic PDEs with high-order accuracy. High-order accuracy is obtained by augmenting the trial function space with singular basis functions. In the case of the nonlinear elliptic PDE that describes capillary singularities, we show that an accurate numerical approximation can be obtained with the finite volume element method through an appropriate change of variable combined with a change of coordinates, motivated by the known asymptotic behaviour. Using this accurate numerical approximation methodology, we can numerically confirm the validity of the known asymptotic expansions in great detail, and we can make two conjectures on asymptotic behaviour of singular capillary surfaces at a cusp for two open cases.

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High-Order Summation-by-Parts Discretization of the Navier-Stokes and Euler Equations

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The compressible Navier-Stokes and Euler equations constitute a formidable set of partial-differential equations (PDEs), the solution of which requires extensive computational resources, particularly if one is interested in optimization of industrially relevant flows. In the early 1970s, Kreiss and Oliger [2] and Swartz and Wendroff [5] demonstrated that substantial efficiency gains are possible using higher-order (HO) methods. In the asymptotic region, HO methods have a local truncation error of order $O([\Delta x]^p)$, where $p \geq 3$, and Δx is the mesh spacing. Thus, for a given accuracy, HO methods require coarser mesh spacing relative to lower-order methods. HO methods have been shown to be more computationally efficient than lower-order methods; some examples are the linear advection equation [6] and the compressible Navier-Stokes (NS) equations [**?**]. Here, we examine discretizations based on HO summation-by-parts (SBP) finite-difference operators, with simultaneous approximation terms (SATs) for boundary and interface treatment, which have been successfully applied to the compressible Euler and NS equations [1, 3].

In conjunction with SATs to weakly impose boundary conditions, SBP operators naturally give rise to multi-block schemes that have constant and, more importantly, low communication overhead, which is advantageous for parallel computations. This results from the fact that only C^0 continuity needs to be maintained between blocks and, regardless of the order of the scheme, the same amount of information is passed between blocks, i.e. there is no need for halo nodes. In curvilinear coordinates, time stability can only be proven for diagonal-norm SBP operators [4]; thus we limit ourselves to those operators. The NS equations require a discrete approximation to the second-derivative with variable coefficients. It is possible to use the application of the first derivative twice, but this results in a large stencil width and reduced accuracy. We will compare and contrast the application of the first derivative twice to SBP operators that have minimum-stencil width on the interior.

Our research deals with aerodynamic optimization; we therefore need a robust and efficient algorithm to solve the compressible NS equations on complex geometries; the SBP-SAT method has proven to be robust and efficient in both direct computations of the NS equations and in the context of the Reynolds averaged Navier-Stokes equations (RANS), see Hicken and Zingg [1], and Osusky and Zingg [3]. Here we will present a suite of test cases, ranging from academic, such as the method-of-manufactured solutions, to practical, such as the NACA-0012 airfoil, to investigate the performance of the proposed operators in the context of laminar flows.

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Parallel High-Order CENO Finite-Volume Method for Large-Eddy Simulation of Turbulent Premixed Flames

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High-order discretization methods offer the potential to significantly reduce the computational costs required to obtain accurate predictions as compared to standard lower-order (second-order) methods. Nevertheless, efficient, universally-applicable, high-order discretizations remain somewhat illusive, especially for more arbitrary three-dimensional and/or unstructured computational meshes and for the prediction of physically complex flows as encountered in large-eddy simulation (LES) of turbulent reactive flows. A novel, parallel, high-order, central essentially non-oscillatory (CENO), cell-centered, finite-volume scheme is proposed for the solution of the Favre-filtered Navier-Stokes equations governing turbulent flows of a fully-compressible reactive mixture and applied to the LES of turbulent premixed flames. The high-order CENO finite-volume scheme of Ivan and Groth [1, 2] for the solution of inviscid and laminar viscous, compressible, non-reactive flows on two-dimensional domains is extended here to the parallel solution of the Favre-filtered LES equations on three-dimensional, multi-block, body-fitted, hexahedral computational mesh. Details of the proposed high-order scheme are discussed and, in order to demonstrate the capabilities of high-order method, LES of a laboratory-scale lean premixed methane-air Bunsen-type flame is considered. For the latter, a flamelet-based subfilter-scale (SFS) LES model is used to describe the unresolved influences of interaction between the turbulence and combustion. The SFS combustion model is based on a presumed conditional moment (PCM) approach in conjunction with flame prolongation of intrinsic low-dimensional manifold (FPI) tabulated chemistry. Comparisons of LES predictions to available experimental data are made and the potential of third- and fourth-order variants of the CENO finite-volume scheme for performing LES of premixed flames is assessed.

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Assessment and Comparison of Discretization Techniques for the Diffusion Operator in High-Order Finite-Volume Methods

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High-order methods are currently being pursued in an effort to reduce the cost of large-scale scientific computing applications such as direct numerical simulations (DNS) and large eddy simulations (LES) of turbulent non-reacting and reacting flows. Among the many challenges raised by the application of high-order schemes to the aforementioned scientific problems, the focus of this talk is on the high-order treatment of diffusive (elliptic) fluxes, which are included in the viscous terms of the Navier-Stokes and other model equations. Unlike the convective fluxes that depend on the solution vector only, the diffusive fluxes also include a dependency on the solution gradient in space. Additionally, the initial data and the diffusion coefficient field may be discontinuous as in the case of the classical diffusive Riemann problem and the heat-conduction problem across the interface between two different materials, respectively.

For the reasons given above, it is very desirable that high-order discretization techniques for diffusive fluxes remain accurate and stable for a variety of initial data and problems while satisfying a maximum principle, even on stretched/distorted meshes. This can be difficult to achieve and even standard lower-order spatial discretization procedures may not possess these characteristics. Nevertheless, several high-order variants have been proposed recently in an effort to arrive at reliable, accurate, and more efficient discretization strategies for the diffusive fluxes.

This talk will consider a detailed assessment and comparison of several treatments for the diffusion operator within the context of a finite-volume discretization scheme. In particular, a multi-dimensional, fourth-order, central essentially non-oscillatory (CENO) finite-volume method is considered [1] and the following approaches for high-order treatment of the diffusive (elliptic) fluxes are examined in this work: (i) the use of a k-order accurate average gradient derived from a $(k+1)$-order accurate reconstruction [1]; (ii) the addition of a penalty term [2] to the average gradient of method (i); and (iii) the use of the solution to the diffusive generalized Riemamn problem [3] in the evaluation of the diffusive fluxes. The predictions of the three approaches are compared and the relative merits of each technique are assessed.

The methods considered are thoroughly assessed based on several test cases for the two-dimensional form of the advection-diffusion equation solved on body-fitted quadrilateral structured grids. These include, but are not limited to, systematic grid convergence studies based on analytical solutions to transient diffusion problems with smooth and discontinuous initial data, to heat conduction problems with discontinuous thermal conductivity, and to convection-diffusion problems characterized by different Péclet numbers.

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An Adaptive High Order Discontinuous Galerkin Solver for Direct Numerical Simulation

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The presentation will discuss our ongoing development of an adaptive high order Discontinuous Galerkin solver for the incompressible Navier-Stokes equations. The DG methodology follows those of [1, 2], recasting the equations in conservation form and employing the internal penalty flux formulation. Approximation spaces are the sets of Lagrangian interpolants of the Legendre polynomials of Nth order (N typically 5-15). Gauss-Lobatto Legendre quadrature is used to evaluate all integrals of the variational formulation on the K elements of the grid.

Adaptation of the DG method is handled as for the Spectral Element method [3] through elemental *a posteriori* error estimators based on the polynomial spectrum of the numerical solution to estimate the elemental error and give an indication of the quality of the solution. The numerical spectrum is fit by least squares to an exponential decay, $e^{-\sigma n}$. $\sigma > 1$ indicates good resolution and hence prescribes p-refinement (i.e. the polynomial order will be increased by 2); $\sigma \leq 1$ indicates poor resolution, and hence h-refinement (i.e. the element will be split in two). Adaptive calculation results are shown below for a scalar advection case. Adaptive Navier-Stokes examples will be shown in the presentation.

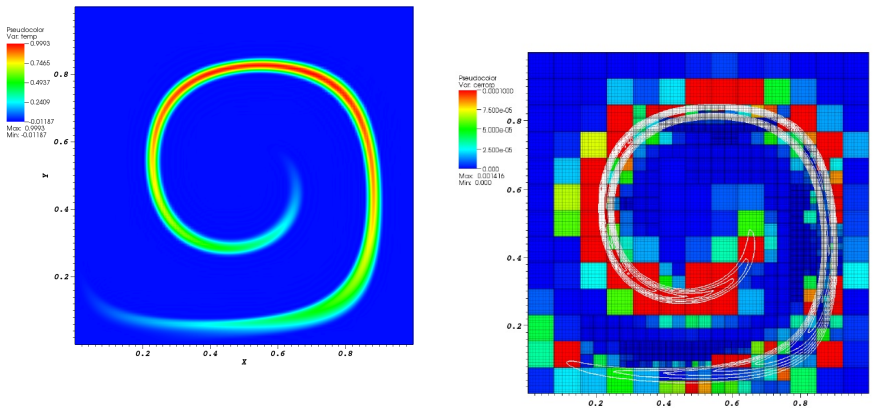

Figure 1: Non-adapted $K = 25 \times 25$, $N = 7$ (left) and h-adapted (right) solution for a scalar advection case. The adapted case started from $K = 13 \times 13$, $N = 9$. The elements are coloured according to the error estimate values.

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Examining nonlinear wave propagation in the trumpet

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Sound production and propagation in brass instruments, specifically the trumpet, will be examined. In particular, the effects of linear and nonlinear wave propagation on the acoustics of the instrument will be discussed. To understand the general behaviour of linear and nonlinear sound waves, experiments were carried out in which simultaneous pressure measurements were taken at various positions along the trumpet. The obtained results will be presented and analyzed. These experiments will help us establish if the nonlinear distortion is strong enough to have musical consequences.

Once the data is reviewed, we will attempt to describe the wave propagation within the trumpet by considering the compressible Euler equations. The system will then be solved by using the discontinuous Galerkin numerical method. The pressure data obtained from the experiments will be used to set up the boundary conditions at the mouthpiece. The numerical results will then be compared with the experimental data to verify how well we were able to describe the nonlinear wave motion within a trumpet.

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Analysis of Heterogeneous Multiscale Methods for Long Time Multiscale Wave Propagation Problems

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Our main goal in this talk is to mathematically investigate the properties of a heterogeneous multi-scale method (HMM) type multi-scale algorithm [1] for approximating the solution of the scalar wave equation over long time

$$\begin{aligned} &\partial_{tt} u^\varepsilon(t,x) - \nabla\cdot(A^\varepsilon(x))\nabla u^\varepsilon(t,x)) = 0, \quad \text{in} \quad [0,T^\varepsilon]\times\Omega, \\ &u^\varepsilon(0,x) = q(x), \quad \partial_t u^\varepsilon(0,x) = z(x), \quad \text{on} \quad \{t=0\}\times\Omega, \end{aligned} \tag{1}$$

with appropriate boundary data. Here $A^\varepsilon(x)$ is a symmetric and uniformly positive definite matrix varying on the small length scale ε, $\Omega \subset R^d$ and $T^\varepsilon \approx O(\varepsilon^{-2})$. As $\varepsilon \to 0$ the numerical approximation of (1) becomes increasingly expensive since all small scales in $A^\varepsilon(x)$ must be resolved over a longer and longer time to obtain accurate results.

HMM is a general framework for efficiently solving this kind of multi-scale problems numerically. A typical HMM algorithm for (1) starts with assuming a macro model $u_{tt} = \nabla\cdot F$ where F represents an unknown flux. The model is discretized on a grid which does not resolve the ε-scale. The missing flux is computed by $F = (\mathscr{K} A^\varepsilon(x) u^\varepsilon_x)$, where $\mathscr{K}$ is an averaging operator in time and space, and u^ε solves the full problem (1) in a domain of size $O(\varepsilon)$, with initial data given by linear interpolation of the current macroscopic state. The computational cost is then independent of ε. For further details of such HMM based methods for the wave equation see [5, 3].

In the analysis of the method we focus on the case when $A^\varepsilon(x) = A(x/\varepsilon)$ with A periodic. For short times $T^\varepsilon = T \approx O(1)$, classical homogenization theory then reveals the limiting behavior of the multi-scale solution and the equation. On the other hand, for long times $T^\varepsilon = O(\varepsilon^{-2})$, the solution $u^\varepsilon(t,x)$ starts to exhibit $O(1)$ dispersive effects which are not present in the short time homogenized solution, [4]. In [2], the short time FD-HMM algorithm from [3] was extended to approximate the solution of long time wave propagation problems. The extension involved only modifying the initial data for the micro problem to a third-order polynomial as well as using a high order averaging kernel $\mathscr{K}$ in the upscaling procedure. Numerical evidences were shown to illustrate that the numerical solution correctly captures the dispersive effects.

In this talk, we give a theoretical foundation for the results in [2], by proving that HMM indeed computes the correct flux also for the long time multi-scale wave problem (1). With suitable macroscale discretization parameters, it will therefore capture the $O(1)$ dispersive effects.

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High-Order Central ENO Finite-Volume Scheme for Ideal MHD

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A high-order accurate finite-volume scheme for the compressible ideal magnetohydrodynamics (MHD) equations is proposed [1]. The proposed high-order MHD scheme is based on a central essentially non-oscillatory (CENO) method [2], combined with the generalized Lagrange multiplier divergence cleaning method for MHD [3].

The CENO method uses k-exact multidimensional reconstruction together with a monotonicity procedure that switches from a high-order (normally fourth-order) reconstruction to a limited low-order reconstruction in regions of discontinuous or under-resolved solution content [2]. Both reconstructions are performed on central stencils, and the switching procedure is based on a smoothness indicator. The proposed high-order accurate MHD scheme can be used on general polygonal grids, and mechanisms to deal with curved boundaries are also described. In particular, structured meshes based on quadrilateral and hexahedral cells are chosen to represent simulation grids.

Several two- and three-dimensional simulations are presented, demonstrating high-order convergence for smooth flows and robustness against oscillations for problems with shocks on logically Cartesian grids. An MHD extension to the Shu-Osher test problem [4] is proposed to assess the capability of the scheme to deal with discontinuities and small-sale flow features at the same time [1]. In two dimensions, the dynamic mesh adaptation capabilities of the approach are demonstrated using adaptive time-dependent simulations of the Orszag-Tang vortex problem with high-order accuracy and unprecedented effective resolution.

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Simulation of the Mixing in An Imploding Shell

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The mixing in a stratified cylindrical shell driven by shock compression is numerically studied using a hybrid method combined with the weighted essentially non-oscillatory shock-capturing method and the tuned center difference scheme, combined with the Runge-Kutta method for time integration. We use the N-species NS equations to simulate the motion. Initial small perturbations with different scales are considered in the simulations. We investigated the mixing according to the mixing zone width and the mixing fraction. It was found that the mixing zone's growth is quite sensitive to the initial perturbation scale, while the atomic mixing degree tends to be independent of the initial perturbation at late time.

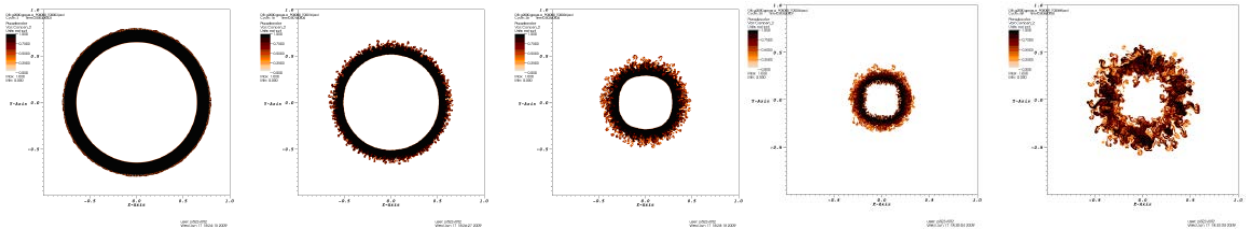

Figure 1: Evolution of the mixing zone.

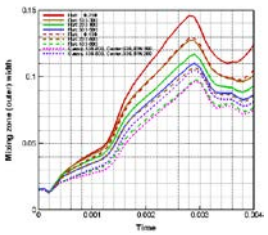

Figure 2: Evolution of the mixing zone.

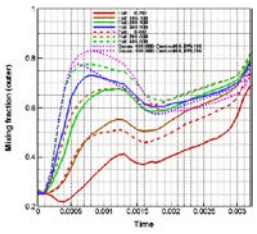

Figure 3: Mixing fraction within the mixing zone.

Fig. 1 shows evolution of the mixing zone in a typical case. Fig. 2 shows the evolution of the mixing zones near the outer interface. We can see that growth of the mixing zone is quite sensitive to the initial perturbation scale. Fig. 3 shows the mixing fraction within the mixing zone, which indicates the atomic mixing degree. We can see that the atomic mixing approaches the asymptotic value of 0.6~0.8 at late time. In this regime, the imprint of initial perturbation tends to be lost as for the atomic mixing degree, although it affects the mixing width.

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Study on Turbulent Mixing Induced by Richtmyer-Meshkov Instability Using the Second-Order Moment Model

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The second-order moment model developed is used to study turbulent mixing induced by Richtmyer-Meshkov instability in the presence of shocks. The transport equations of Reynolds stresses, turbulent mass flux and density variance are used to consider density fluctuations and turbulence anisotropy. Third-order Runge-Kutta method is used to carry out time integration. Advection terms use high order WENO method to reconstruct fluxes on grid boundaries. Alternate direction implicit (ADI) method is used to solve diffusion terms. On the basis of these, shock tube experiment carried out by Poggi in CEA (see Refs. [1]) is simulated. In this experiment laser Doppler anemometer (LDA) was used to measure instantaneous velocities of gas mixture in shock tube and the evolution of velocity fluctuations was obtained before and after the interaction of turbulent mixing zone (TMZ) with the reflected shock wave. It is this experiment that first gives direct measurement of turbulence, which provides data to validate turbulent mixing models. The calculation results are compared with detailed experimental data. It was found that the present model is able to calculate turbulence amplification by multiple shock waves in the presence of large density gradients due to mixing and turbulence anisotropy in TMZ (see Refs. [2]). These results indicate that the model closure, model constants, numerical algorithm and the implementation of the model used in the paper are proper. Moreover the influences of shock Mach number and Atwood number on turbulent mixing are further investigated (see Refs. [3, 4]).

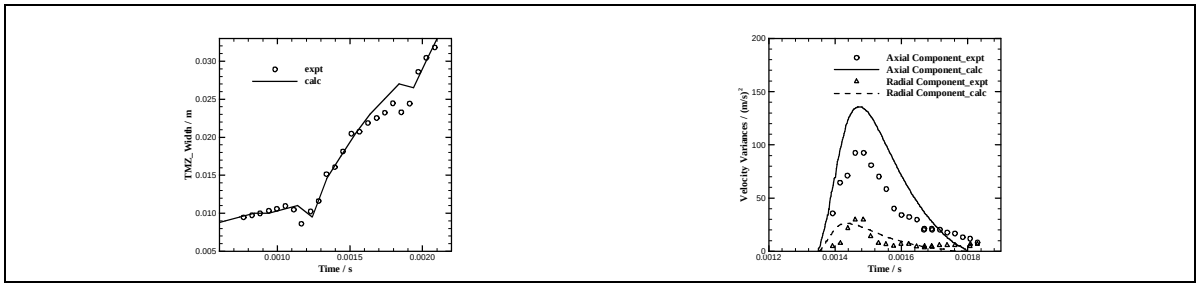

Figure 1: Evolution of the width of TMZ and the axial and radial components of the Reynolds stress tensor at X=169mm

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Recent Progress in Hyperbolic Problems: Theory and Computation (SS-HPTC)

Organizers:
Jae-Hun Jung (SUNY University at Buffalo)
Lilia Krivodonova (University of Waterloo)
Allen Tesdall (CUNY College of Staten Island)

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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High Order Limiters for Hyperbolic Equations

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The challenge of producing solutions that have both high order accuracy and are physically realistic. This paper describes recent advances amde in connection with Essentially Non-Oscillatory (ENO) methods and Weighted Essentially Non-Oscillatory (WENO) methods that are of fundamental importance in the numerical solution of hyperbolic equations. A key property of such equations is that the solution must remain positive or lie between bounds. A modification of the polynomials used in ENO methods to ensure that the modified polynomials are either bounded by adjacent values (data-bounded) or lie within a specified range (range-bounded) is considered.

A key problem in the case of these methods is to bound the derivatives of the ENO reconstruction function (or a number of such polynomials). A recent method of Zhang and Shu offers a way to do this. In this talk we show that there is an alternative approach that is potentially attractive.

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On the solution of dispersive evolution equations with discontinuous data

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We discuss the behavior of solutions of initial-value problems for linear evolution equations when the initial conditions are discontinuous. In particular, by formulating appropriate asymptotic expansions at small times, we show how such discontinuities influence the behavior of the solutions. We then discuss the behavior of solutions of initial-boundary value problems, where we investigate the role of the boundary conditions and of the compatibility conditions between initial data and boundary data, and we obtain a precise characterization of the corner singularities that arise when these compatibility conditions are not satisfied. Finally, we briefly mention the consequences of these results on the behavior of initial value problems and initial-boundary value problems for dispersive nonlinear evolution equations.

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An Efficient Implicit Boundary Integral Solver for the Vlasov-Maxwell System

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Maxwell's equations are an integral part of many plasma models, and therefore robust, efficient solvers are needed in order to attain accurate numerical simulations of plasma. By formulating the Vlasov-Maxwell problem in terms of vector potentials, Maxwell's equation reduces to 4 wave equations, (one for the scalar potential and 3 for the vector potential), forced by the charges and currents as determined by the electron and ion distribution functions. Such problems are challenging because they often involve multiple time and spatial scales, complex geometries, and many particles, which are modeled as moving point sources. Explicit methods are efficient for spatial discretization, but can only take small time steps due to the CFL restriction, and are therefore are unfavorable for long time simulations.

We present an implicit, A-stable boundary integral solver (IBIS) for the wave equation, using a method of lines transpose (MOL^T) approach. We first build a fast O(N) solver in one spatial dimension, and then extend it to higher dimensions using alternate direction implicit (ADI) splitting, thus maintaining efficiency. This makes our IBIS as efficient as explicit solvers, but additionally allows for larger time steps and thus faster simulations. We can also address complex geometries, moving point sources, and a wide variety of boundary conditions. Additionally, we have implemented domain decomposition, which makes our algorithm flexible for use in adaptive mesh refinement.

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The design of a class of positivity preserving high order Lagrangian schemes for multi-material compressible flow

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Robustness of schemes has raised an increasing interest among the community of computational fluid dynamics. One mathematical aspect of scheme robustness is the positivity preserving property. At high Mach numbers, solving the conservative Euler equations can lead to negative densities or internal energy. In this talk, we construct uniformly high order accurate conservative Lagrangian schemes which preserve positivity of density and internal energy for Euler equations solving multi-material ideal and non-ideal compressible flow. We first develop a approximate Riemann solver for the Lagrangian scheme which can preserve the positivity of density and internal energy in the simulation of the multi-material flow with the general equation of state. Then we design a class of high order positivity preserving Lagrangian schemes by using the essentially non-oscillatory (ENO) reconstruction, the strong stability preserving (SSP) high order time discretizations and the positivity preserving limiter which can be proven to maintain uniformly high order accuracy and is easy to implement. One-dimensional and two-dimensional numerical tests for the high order Lagrangian scheme are provided to demonstrate the effectiveness of the method.

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Fast Sweeping Methods for Steady State Problems for Hyperbolic Conservation Laws

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In this talk, I will discuss several simple fast sweeping methods to approximate the steady state solutions of hyperbolic conservation laws. The original fast sweeping methods were developed for stationary Hamilton-Jacobi equations. The methods rely on numerical Hamiltonian, Gauss-Seidel type nonlinear iterative method, and a finite number of sweeping directions to compute the stationary viscosity solution efficiently. We extend the fast sweeping methods to solve hyperbolic conservation laws with source terms. By incorporating the numerical flux, we developed efficient methods which can capture correct stationary viscosity solutions even when discontinuities appear. Extensive numerical examples in both scalar and system of equations in one-, and two-dimensions illustrate the efficiency and accuracy of the new approach. Multigrid framework could also be applied to accelerate the convergence of the iterations.

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Fast recovery of far-field time-domain signals from near-field data

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Time-domain simulation of linear hyperbolic PDEs on a finite computational domain requires the introduction of a fictitious outer boundary. A long standing challenge in the computation of waves is to identify the far-field or asymptotic signal. From data $\psi(t,r_1)$ recorded on a sphere defined by r_1 we seek to recover the far-field signal $\psi(t+(r_2-r_1),r_2)$ which would reach large distances r_2 including infinity. Far-field signals are especially important as they encode information about the physical system.

In this talk I show how far-field signal recovery is handled via a time-domain convolution

$$\psi(t+(r_2-r_1),r_2) = \int_0^t \phi(t-t',r_1,r_2)\psi(t',r_1)dt' + \psi(t,r_1) \tag{1}$$

of the solution recorded on a sphere r_1 with a well-defined kernel $\phi(t-t',r_1,r_2)$. A kernel which describes signal recovery for the ordinary (acoustic) wave equation can be written in closed-form. Using rational approximation techniques developed by Alpert, Greengard and Hagstrom [1] this kernel can be "compressed" as a compact sum-of-poles in the frequency domain. Whence the far-field signal is given by convolution

$$\psi(t+(r_2-r_1),r_2) = \sum_{k=1}^{\ell} \gamma_k \int_0^t \mathrm{e}^{\beta_k(t-t')}\psi(t',r_1)dt' + \psi(t,r_1) \tag{2}$$

with a small number of damped exponentials. In the limit $r_2 \to \infty$ we call Eq. (2) *asymptotic-waveform evaluation*.

For linear hyperbolic PDEs where one does not know a closed-form kernel representation the AGH technique permits signal recovery to be written in the form of Eq. (2) without loss of accuracy. We use asymptotic-waveform evaluation to compute signals generated from binary black hole systems modeled by the Regge-Wheeler-Zerilli equations as well as signal "teleportation" between two finite (smaller) radial values [2].

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Hyperbolic Descriptions of Viscous Heat-Conducting Gaseous Flows and Their Solution

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The use of fully hyperbolic moment closures for the numerical prediction of gaseous flows provides several immediate advantages. The closures lead to transport equations for an extended set of macroscopic quantities or moments that provide descriptions of both near-equilibrium and more general non-equilibrium flows. The moment equations are potentially valid from the continuum limit, through the transition regime, up to and approaching the near-collisionless or free-molecular flow limit. This is in contrast to traditional fluid-mechanic descriptions, such as the Euler and Navier-Stokes equations, which are only valid in or near local equilibrium and are therefore inappropriate for situations with significant deviations from equilibrium. In addition to the modelling advantages, hyperbolic moment closures present many numerical advantages. Moment closures are much less expensive than particle simulation techniques commonly used to described non-equilibrium gaseous flows , particularly for near-continuum and low-speed flows. Moreover, the first-order nature of moment equations allows for the prediction of viscous or heat-transfer effects without the need for the evaluation of second derivatives (this is in direct contrast to the Navier-Stokes equations). Numerical solutions to first-order hyperbolic equations are less sensitive to grid irregularities that often result from adaptive-mesh-refinement or embedded-boundary techniques [1]. Removing the requirement for the discretization of higher than first-order derivatives also means that numerical solution schemes can gain an extra order of spatial accuracy for the same reconstruction stencil when compared to descriptions requiring the discretization of second-order derivatives. Many numerical schemes are well-suited to the solutions of hyperbolic partial-differential equations, including upwind Godunov-type finite-volume and discontinuous-Galerkin schemes. While accurate solution methods have also been developed for equations have an elliptic and/or parabolic nature, the development of schemes that handle conservation equations of mixed type with equal elegance has proven to be significantly more of a challenge.

Recently, McDonald and Groth [2] and McDonald and Torrilhon [3] have proposed novel hyperbolic moment closures for describing both viscous and heat-conducting non-equilibrium gaseous based on maximum-entropy formulations having desirable mathematical features, including a well-defined entropy and strictly hyperbolic moments equations for a wide-range of realizable moments. The numerical solution of these hyperbolic closures using finite-volume methods with block-based adaptive mesh refinement (AMR) on multi-block, body-fitted, computational mesh is discussed with application to a number of canonical non-equilibrium flows, including channel flows, flow past a sphere, and stationary shock-wave structure.

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Normal forms and a Burgers-Hilbert equation

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The Burgers-Hilbert equation arises as a model equation for the motion of a vortex patch or discontinuity in a two-dimensional, inviscid, incompressible fluid flow, and describes the effect of nonlinear steepening on an interface or wave that oscillates at a constant background frequency. For small amplitudes, these oscillations delay wave breaking. We will explain how non-standard normal form methods can be used to prove an enhanced life-span of small smooth solutions of the Burgers-Hilbert equation in comparison with the inviscid Burgers equation. These normal form methods can be applied to other quasilinear wave equations, for which the Burgers-Hilbert equation provides a useful test case. This is joint work with M. Ifrim, D. Tataru, and D. Wong.

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Two dimensional water waves in holomorphic coordinates

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This article is concerned with the infinite bottom water wave equation in two space dimensions. We consider this problem expressed in position-velocity potential holomorphic coordinates. Viewing this problem as a quasi-linear dispersive equation, we establish two results: (i) local well-posedness in Sobolev spaces, and (ii) almost global solutions for small localized data. Neither of these results are new; they have been recently obtained by Alazard-Burq-Zuily, respectively by Wu using different coordinates and methods. Instead our goal is improve the understanding of this problem by providing a single setting for both results, as well as new, somewhat simpler proofs.

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A Fourth-Order Solution-Adaptive CENO Scheme for Three-Dimensional Multi-Block Cubed-Sphere Grids

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High-order accurate and efficient computational methods are highly desirable in many fields of computational physics, particularly for large-scale scientific computing applications such as high-fidelity modelling of turbulent non-reactive and combusting flows, numerical computation of electromagnetic flows, and computational aeroacoustics. Standard spatial discretizations (i.e., methods up to second order) can exhibit excessive numerical error and are therefore very often not practical for these applications. Improved numerical efficiency may be achieved by raising the order of accuracy of the spatial discretization. Adaptive mesh refinement (AMR) can also minimize the computational cost of numerical simulations, by automatically adapting the computational grids to the solution of the governing equations. For numerical simulations of physically complex flows characterized by a wide range of spatial and temporal scales both high-order discretizations and AMR are demanded. Moreover, these approaches require an effective parallel implementation so as to run on thousands of computing cores efficiently.

Cubed-sphere grids [1] have recently gained increasing popularity for simulating fluid flows in spherical shell domains that naturally occur in the modelling of problems from fields as diverse as climate and weather modelling, space physics, astrophysics, and geophysics. Thus, scalable high-performance algorithms capable of reducing the time required to obtain numerical solutions of these problems on various cubed-sphere grids are highly desirable.

This work considers the development and application of a fourth-order accurate, central essentially non-oscillatory (CENO) finite-volume scheme [2] for hyperbolic conservation laws on several configurations of three-dimensional (3D) cubed-sphere grids. The multi-dimensional approach uses k-exact reconstruction together with a monotonicity procedure that switches between high-order and low-order reconstruction based on a smoothness indicator. Hexahedral cells with trilinear faces are employed to handle nonplanar cell faces, achieving uniform high-order accuracy throughout the cubed-sphere grid. Furthermore, the degeneracies arising at the corners between adjacent sectors of the cubed-sphere grid are treated in a consistent manner, thereby allowing the extension of the proposed algorithm to various multi-block cubed-sphere grids. The 3D CENO scheme is implemented in a parallel, dynamically solution-adaptive, simulation framework [3].

Several applications of the proposed high-order accurate numerical procedure to prediction of compressible flows on cubed-sphere grids are presented. These include, but are not limited to, thorough assessments of the numerical scheme to demonstrate high-order accuracy based on systematic grid convergence studies, and simulations of flows containing shocks to illustrate algorithm robustness. Furthermore, the talk will present parallel performance studies and demonstration of the effectiveness of the AMR algorithm.

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Two-dimensional Riemann problems for conservation laws and shock reflection

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We give an overview of the free boundary techniques used in analysis of two-dimensional Riemann problems describing shock reflection for several systems of conservation laws. Our main example is the system of isentropic gas dynamics equations

$$\begin{aligned} &\rho_t + (\rho u)_x + (\rho v)_y = 0, \\ &(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0, \\ &(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0, \end{aligned} \tag{1}$$

where ρ stands for density, u and v are velocities in x and y directions, respectively, and p is pressure. We also consider simpler models such as unsteady transonic small disturbance equation (UTSDE) and the nonlinear wave system (NLWS). The UTSDE, NLWS and system (1) are prototypes of the full Euler gas dynamics equations and their importance in the study of the shock reflection problems was discussed in [2, 8]. In each case, we discuss the Riemann initial data resulting in regular shock reflection (transonic and supersonic).

We use the approach given in [4] on the study of steady transonic small disturbance equation, which was later adopted to the UTSDE and NLWS (some references are [1, 3, 6, 7]. The main idea is to rewrite the problem in self-similar coordinates $\xi = x/t$ and $\eta = y/t$ which leads to a free boundary problem of mixed hyperbolic-elliptic type. The free boundary is the reflected shock, whose position, through Rankine-Hugoniot conditions, depends on the solution. The interactions in the hyperbolic part are resolved using the theory of one-dimensional hyperbolic conservation laws. The solution in the elliptic part is described using a second order elliptic equation for one of the variables with mixed (Derichlet and oblique-derivative) boundary conditions. Its existence is studied using various fixed point theorems and Schauder estimates from [5].

Existence of solutions to Riemann problems for UTSDE and NLWS leading to both transonic and supersonic regular shock reflections was proved (see [1, 3, 6, 7]), and we discuss challenges arising in the study of system (1).

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On Isentropic Flow with Large Data

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We consider one-dimensional compressible flow of a gas as described by the isentropic Euler system in a Lagrangian frame (t,X) by

$$\tau_t - u_X = 0 \tag{1}$$
$$u_t + p(\tau)_X = 0, \tag{2}$$

where $\tau = \rho^{-1}$ denotes specific volume, u is particle velocity, and $p(\tau) \propto \tau^{-\gamma}$ is pressure ($\gamma \geq 1$).

Despite its simplicity this model is not well-understood mathematically. Given the role played by a priori variation bounds in Glimm's small variation theory, it is natural to ask if "large" solutions to (1)-(2) admit similar estimates. We present examples showing that certain types of variation bounds are *not* available for (1)-(2). The examples rely on the singular behavior of the system near vacuum.

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An Adaptive RBF-WENO Reconstruction Method for Hyperbolic Problems

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We present an adaptive RBF-WENO method using the multi-quadric RBFs for the local reconstruction. The method is that the shape parameters are adaptively determined based on the regularity of the local reconstruction in each stencil. By this flexibility, the reconstruction can enhance accuracy and convergence although using polynomials in each stencil allows only a fixed convergence rate. We construct the ENO and then WENO reconstructions and show how the accuracy is enhanced with numerical examples.

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Relaxing the CFL Number of the Discontinuous Galerkin Method

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Discontinuous Galerkin methods (DGM) have a Courant-Friedrichs-Lewy (CFL) number decreasing with the increase of the order of approximation p for convection dominated problems. This makes them computationally more expensive when compared with finite volume or finite difference methods. We propose a modification of the scheme that results in a family of high order methods which have a less restrictive CFL number. We show that in the standard DG method the dispersion and dissipation errors and the spectrum of the semi-discrete scheme are related to the $[p/p+1]$ Pade approximation of $exp(z)$ and $exp(-z)$. This Pade approximant is responsible for both the superconvergent error in diffusion and dispersion ($O(h^{2p+2})$ and $O(h^{2p+3})$, respectively) and the small CFL number. We propose to modify the DGM so that the resulting rational approximation of the exponent corresponds to a spatial discretization operator with a smaller spectrum, i.e. a less restrictive CFL number. This is achieved by scaling the amount of the numerical flux contribution to the equations evolving solution coefficients in time. For the considered orders of approximation, the improvement in the CFL number ranges between two and five fold depending on how much modification is brought into the scheme. The interesting aspect of the new schemes is that the $(p+1)$st rate of convergence in the L^2 norm as well as the compact stencil of the traditional DGM are preserved. We show that for the same amount of work the new schemes are more efficient for smooth problems and considerably more accurate for problems with discontinuities.

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Nonlinear wave interaction for the ultra-relativistic Euler equations

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We study the ultra-relativistic Euler equations for an ideal gas and present the solution of the Riemann problem, which is free from vacuum. We introduce a new function, which measures the strengths of the waves of the ultra-relativistic Euler equations, and use it to derive sharp estimates for the wave interactions.

Our study of interaction estimates allows us to determine the type of the outgoing Riemann solutions. From this study we were able to derive a new front tracking technique for the ultra-relativistic Euler equations, which gives exact weak solutions.

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Sparse spectral methods for helically symmetric gravitational binaries

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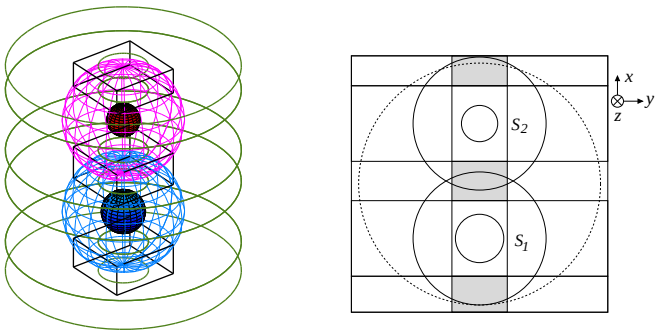
We describe ongoing work intended to solve the helically symmetric Einstein equations (or post-Minkowski approximations thereof) for binary configurations, such as two neutron stars. Helically symmetric solutions may serve as a platform for constructing improved initial data for the hyperbolic evolution problem of general relativity, in particular removing the typical (but physically incorrect) assumption of conformal flatness. We employ sparse modal spectral methods based on the technique of "integration preconditioning" [1], and a key focus of our work involves practical extension of the technique to higher dimensions and multiple subdomains.

The model problem involves the 3d helically reduced wave equation: $L\psi = g$ on $\mathscr{D}$ with Dirichlet boundary conditions at $\partial S_1^- \cup \partial S_2^- \subset \partial\mathscr{D}$ and radiation boundary conditions at $\partial S_3^+ \subset \partial\mathscr{D}$ (see the figure). Here $L = \partial_x^2 + \partial_y^2 + \partial_z^2 - \Omega^2\left(x\partial_y - y\partial_x\right)^2$ is the "helical Laplacian" (with rotation rate Ω) and g is a prescribed source. As described in [2] this mixed-type problem arises via helical reduction of the inhomogeneous 3+1 wave equation. The helical reduction of the Einstein equations described in [3, 4] involves a tensorial field resolved into ten coupled "helical scalars" $\psi^{(\alpha\beta)}$ each of which obeys a copy $L\psi^{(\alpha\beta)} = g^{(\alpha\beta)}$ of the above equation. However, for this formulation $g^{(\alpha\beta)}$ is now not an external source; rather it is a nonlinear coupling function of the helical scalars which does include second-order derivative terms (albeit of quadratic smallness). This talk will focus on the simplest helical neutron star model.



(a) 3d view of domain decomposition. (b) Cross-sectional view.

Figure 1: DECOMPOSITION OF $\mathscr{D}$. The inner configuration of 10 rectangular, cylindrical, and spherical subdomains (S_1 and S_2) is enclosed within an outer spherical shell S_3 (not shown save for its inner boundary in (b)). $\partial S_k^{\pm}$ denotes the outer/inner boundary of S_k for $k = 1, 2, 3$.

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The Dynamics of a Scalar Field in Anti-de Sitter

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The gravitational collapse of a scalar field in spherically symmetric spacetime serves as an ideal problem for exploring the nonlinear aspects of gravity because of its relative simplicity and its interesting behavior. One well known example is black hole (BH) critical phenomena found by Choptuik [1] revealing interesting nonlinear behavior at the threshold for BH formation. He found this threshold by conducting a bisection search on the initial amplitude of a scalar field evolving within an asymptotically flat spacetime. For some initial data family characterized by a critical parameter, say p^*, initial data with $p > p^*$ formed a BH while initial data with $p < p^*$ dispersed to infinity.

Studying the scalar field instead in Anti-de Sitter (AdS), Refs. [2, 3] found that even nominally subcritical ($p < p^*$) initial data eventually, and inevitably, collapsed as well. AdS has the remarkable property that its boundary is in causal contact with its bulk, and one effect of this is that an initial pulse that does not form a BH will eventually reflect from the boundary at infinite radius. The numerical evolutions of [2, 3] suggested that even the weakest initial pulse will, after some huge number of reflections, sharpen (via a *weakly turbulent instability*) to the point where the energy density collapses to BH formation.

Here, I discuss recent work [4, 5, 6] studying a complex scalar field in spherically symmetric AdS. Our work reproduces the work of [2, 3], and studies the focusing mechanism by which the bulk energy density cascades to shorter scales. We also introduce a reflecting boundary condition at finite radius and find similar BH formation after repeated bounces. Assuming a stationary ansatz for the complex field, we find boson star solutions. Adopting such solutions along with an appropriate perturbation as initial data, we evolve and study the nonlinear stability of boson stars.

We argue that this instability of AdS to BH formation results from the nonlinear self-gravity of the scalar pulse, and that the casually connected boundary of AdS allows for the self-gravity to act continuously. This simple explanation requires some augmentation in light of a few surprises encountered: (i) The introduction of an artificial reflecting boundary condition introduces a limit below which sufficiently weak initial data fails to produce a BH, (ii) sufficiently weak perturbations of a boson star appear to propagate without sharpening and without eventual BH formation, and (iii) evolutions suggest that a large class of initial data, not just that of stationary solutions, is immune to this turbulent instability.

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Absorbing boundary conditions for quantum relativistic mechanics

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Microlocal analysis is used to derive pseudo-differential transparent and absorbing boundary conditions for the 1-d and 2-d Klein-Gordon and Dirac equations modeling quantum particles subject to classical electromagnetic fields.

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Challenging simulations of Black Hole Binaries

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We review the full numerical techniques that allow to simulate binary black holes by solving General Relativity field equations. We describe the specific techniques used to deal with the most challenging cases of small mass ratio binaries [1], highly spinning black holes [2], and large separation binaries [3].

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Exponential time integration methods for wave-dominated problems

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We present our recent studies on exponential time integration methods for solving wave-dominated problems arising in electromagnetics and fluids [1, 2]. We discretize the spatial domain based on a high-order spectral-element discontinuous Galerkin approach. From the resulting semi-discrete form, we can obtain our approximate solution analytically, expressed by a large matrix exponential. We project the large matrix exponential onto a small dimension of Krylov subspace by the Arnoldi process [3] and compute the matrix exponential of the resulting Hessenberg matrix in a small dimension m.

For computing the matrix exponential, we obtain eigenvalues of the Hessenberg matrix of dimension $m \times m$ using available library packages and perform ordinary exponential function operations for the eigenvalues. The scheme involves mainly matrix-vector multiplications, with the rate of convergence $O(\Delta t^{m-1})$ so that it allows taking a larger timestep size as m increases.

We demonstrate practical implementation of the algorithms including the accuracy and computational cost. Case studies are presented for electromagnetic waveguide problems, Schrödinger solutions, and lattice Boltzmann method approach for fluids simulations.

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Compressible Navier-Stokes equations with temperature dependent dissipation

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From its physical origin, the viscosity and heat conductivity in compressible fluids depend on absolute temperature through power laws. The mathematical theory on the well-posedness and regularity on this setting is widely open. I will report some recent progress made on this direction, with emphasis on the lower bound of temperature, and global existence of solutions in one or multiple dimensions. The relation between thermodynamics laws and Navier-Stokes equations will also be discussed. This talk is based on joint works with Weizhe Zhang.

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Estimation and propagation of volcanic source parameter uncertainty and the Eyjafjallajökull plume

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The 2010 eruption of the Eyjafjallaj/"okull volcano wrecked havoc for European aviation. To make predictions of the likely position of the ash cloud and issue advisories to the airline industry, the London Volcanic Ash Advisory Center used mathematical models of advection and dispersion. These models require input data on volcanic source conditions such as eruption column height and mass loading, which are usually not well constrained. The outputs of these models also depend on other input data such as varying winds, which have stochastic variability. Estimates of all these uncertain inputs is needed in order to make probabilistic predictions of ash cloud motion.

There has not been a systematic study of these variable and uncertain source inputs, and the consequent probabilistic output forecasts. This presentation examines the forecasting problem, accounting for both uncertain and stochastic inputs. At the same time, it can be important for geo-scientists to study the inverse problem – using cloud location to estimate source parameters; the presentation also discusses methodologies that can be used to solve this inverse problem.

At the core of our approach is a marriage of a model of a volcanic eruption column, called BENT, with an advection and dispersion code, PUFF. BENT uses physical features such as the diameter of a volcanic vent and the sizes of ejected particles to predict the structure of an eruption column. This column structure is then used as input to PUFF, which propagates the ash cloud.

In performing the uncertainty quantification calculations, techniques from generalized polynomial chaos and from conjugate unscented transform are used. Careful attention is given to convergence issues, particularly regarding the PUFF code.

For validation, the BENT-PUFF propagation predictions are compared with the documented motion of the Eyjafjallaj/"okull ash cloud.

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Special Solutions in Smectic Electroconvection

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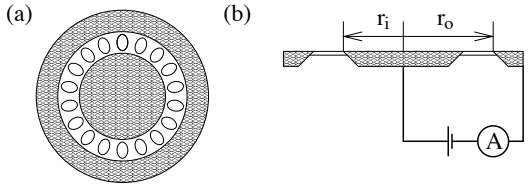
We discuss electroconvection in a free submicron-thick liquid crystal film in an annular geometry. Figure (a) shows the experimental apparatus from above. The inner and outer dark regions denote electrodes between which a voltage difference is imposed. Between them is the annular film with circles denoting the convection cells of charge that form when the voltage difference is sufficiently large. Figure (b) shows the apparatus from the side.



Because of the annular geometry, the dynamics are periodic in the azimuthal direction and the only boundaries are those at which the convective forcing is applied. The liquid crystal is in smectic A phase, forming a nearly-perfect two-dimensional fluid because the film does not change thickness, even while flowing. Also, the inner electrode can be rotated and so the experiment can be used to study the interplay between a stabilizing force applied via the boundary (Couette shear) and convection. We present preliminary numerical simulations of special solutions such as convection cells, oscillatory convection cells, undulating convection cells, and localized vortex solutions.

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Linear Stability Analysis of the Discontinuous Galerkin Method on Uniform and Nonuniform Grids

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Applying a discontinuous Galerkin spatial discretization to a hyperbolic PDE results in a system of ODEs for the unknown solution coefficients. This system can be solved with a time integration scheme such as a Runge-Kutta method. The largest allowable time step depends on the eigenvalues of the spatial discretization matrix and the absolute stability region of the ODE solver. In this talk we present an analysis of the eigenvalues of the DG scheme with the upwind flux applied to the one-dimensional scalar advection equation. We derive a formula for the eigenvalues on an N element uniform grid in terms of the sub-diagonal [p,p+1] Padé approximation of exp(-z), where p is the order of the finite element basis. This allows us to draw a number of conclusions about the CFL number and stability of the scheme. For example, we obtain a bound on the largest in magnitude eigenvalue and also its asymptotic growth rate with the order of approximation. Then, we analyze the eigenvalues of the DG method on nonuniform grids and demonstrate that a CFL condition less than the one prescribed by the local stability condition (and commonly assumed) can be used.

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Smoothness Increasing Accuracy Conserving (SIAC) filtering for discontinuous Galerkin approximations to nonlinear hyperbolic conservation laws

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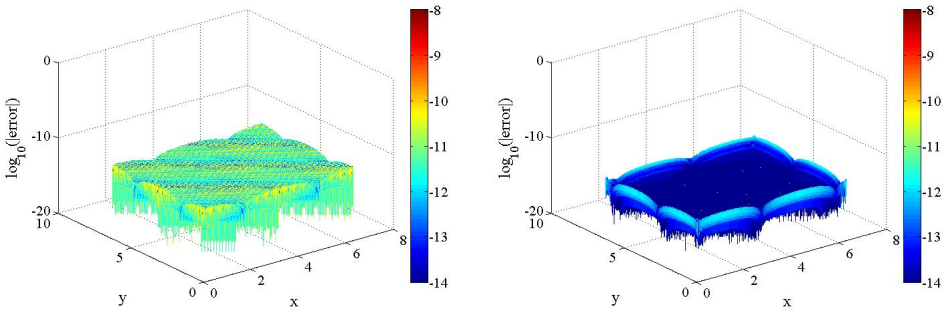
In this presentation we discuss the application of a Smoothness-Increasing Accuracy-Conserving (SIAC) filtering to discontinuous Galerkin (DG) approximations for the solution to scalar nonlinear hyperbolic equations. The SIAC filter can increase the order of accuracy of the DG approximation from $k+1$ to $2k+1$ for time-dependent linear hyperbolic partial differential equations solved over translation invariant meshes (here k refers to the highest degree polynomial used in the approximation). Additionally, performing such filtering rids the approximation of oscillations in the error, as shown in Figure 1. The SIAC filtered DG solution is obtained by convolving the DG approximation with a convolution kernel consisting of a linear combination of B-splines.

In this talk we discuss the barriers to extending this technique to nonlinear hyperbolic equations. That is, in order to make SIAC filtering applicable to nonlinear hyperbolic equations, we must establish both the proper error estimates in the negative-order norm for smooth regions as well as one-sided filtering for treating boundaries and shocks. We demonstrate computationally and theoretically that it is possible to obtain $2k+m$, where m depends upon the flux for the DG solution [1]. Further, we show that by a suitable modification of the filtering kernel near the boundary or shock regions, we are able to conserve, and in most cases improve, accuracy and smoothness [2].



(a) DG Error (b) Post-processed

Figure 1: Comparison of the point-wise errors in log scale of the (a) DG solution and (b) the SIAC filtered solution using basis polynomials of degree $k = 4$, mesh 80×80.

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Effects of Nonstrict Hyperbolicity on Singularity Formation

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We examine a 2x2 genuinely nonlinear hyperbolic system involving (e,p) variables which loses the property of strict hyperbolicity along sets in the (x,t) plane where $e=0$. If the initial condition $e_0(x)$ is set to be increasing function with $e_0(0)=0$, then along the line $x=0$ we have $e(0,t)=0$ for $t>0$. It was established in earlier work ([1]) that a singularity forms in finite time along $x=0$, even in the presence of damping. That is, unlike for the case of strictly hyperbolic systems, dissipation is not strong enough to preserve smoothness of small solutions globally in time. Under the conditions that $e_0'(0)>0, p_0''(0)<0$ and $(p_0''(0))^2-(e_0'(0))^4>0$, the hyperbolically degenerate set along $x=0$ bifurcates from a point $(0,t^*)$ to create a secondary curve prior to blowup. Thus there exists an additional curve $L: t=\psi(x)$ crossing $x=0$ at $t=t^*$ along which characteristic speeds are equal and $e=0$. We will analyze the consequence of this phenomenon and provide properties of the curve L. Some examples of solutions will be presented for the case of no damping.

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A Generalized Sign-Changing Liouville Equation

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We examine singularity formation in the Goursat and 'mean-Goursat' problems for spatially periodic solutions to the sign-changing Liouville equation

$$\partial_{t\alpha} \ln u = f(\alpha) u^{\lambda}, \ t > 0, \tag{1}$$

with solutions having initial data

$$u(\alpha, 0) = g(\alpha), \tag{2}$$

and satisfying either

$$i) \ u(0,t) = h(t), \ \text{ or } \ ii) \ \int_0^1 u(\alpha,t) d\alpha = k(t), \ t > 0, \tag{3}$$

for given positive functions g and h or k. The requirement of having spatially periodic solutions places change of sign as a necessary condition on the function f.

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A numerical investigation into high-order multiderivative integrators for hyperbolic conservation laws

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We advocate the use of seldom seen multiderivative time integrators for hyperbolic conservation laws because they work well with modern computer architectures. When compared with traditional (single-derivative) Runge-Kutta methods, the primary advantages multiderivative methods have are twofold: first, they naturally contain a low memory footprint, and second, they require less computational effort in terms of number of Riemann solves and number of WENO reconstructions.

Multiderivative methods are similar to Taylor methods because they evaluate higher derivatives of the function in order to attain high-order accuracy, and the multistage versions of these methods are similar to (single-derivative) Runge-Kutta methods because they add extra stages in order to increase the overall order of accuracy. Recent work on applying multiderivative time integrators to hyperbolic conservation laws presented a single, fourth-order method as its model multiderivative example [1]. There, they demonstrated how a multiderivative method could be used to solve hyperbolic problems using WENO and discontinuous Galerkin spatial discretizations. Their work presented results for numerous test problems that indicate multiderivative methods compete well with popular high-order strong stability preserving time integrators.

In this work, we present a numerical investigation into results for higher-order two-derivative Runge-Kutta methods that use extra stages [2]. For a spatial discretization, we use seventh and ninth-order WENO methods, and we compare results with popular high-order time integrators. In addition, we present 2D results that use a multiderivative discontinuous Galerkin formulation.

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Glancing weak Mach reflection

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We study the glancing limit of weak shock reflection, in which the wedge angle tends to zero with the Mach number fixed. Lighthill showed that, according to linearized theory, the reflected shock strength approaches zero at the triple point in reflections of this type. To understand the nonlinear structure of the solution near the triple point in nearly glancing reflections, then, it is necessary to understand how the reflected shock diffracts nonlinearly into the Mach shock as its strength approaches zero. Towards this end, we formulate a half-space initial boundary value problem for the unsteady transonic small disturbance equations that describes nearly glancing Mach reflection. We solve this IBVP numerically, and we find in the solutions a complex reflection pattern that closely resembles Guderley Mach reflection. This is joint work with John Hunter.

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Conservation Laws with no Classical Riemann Solutions: Existence of Singular Shocks

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The basic tool in the construction of solutions to the Cauchy problem for conservation laws with smooth initial data is the Riemann problem. In this talk I will review the results obtained for the solutions to the Riemann problem and present a system of two equations derived from isentropic gas dynamics with no classical solution. I will then use the blowing-up approach to geometric singular perturbation problems to show that the system exhibits unbounded solutions (singular shocks) with Dafermos profiles.

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Shock detection of discontinuous Galerkin methods using multiwavelets

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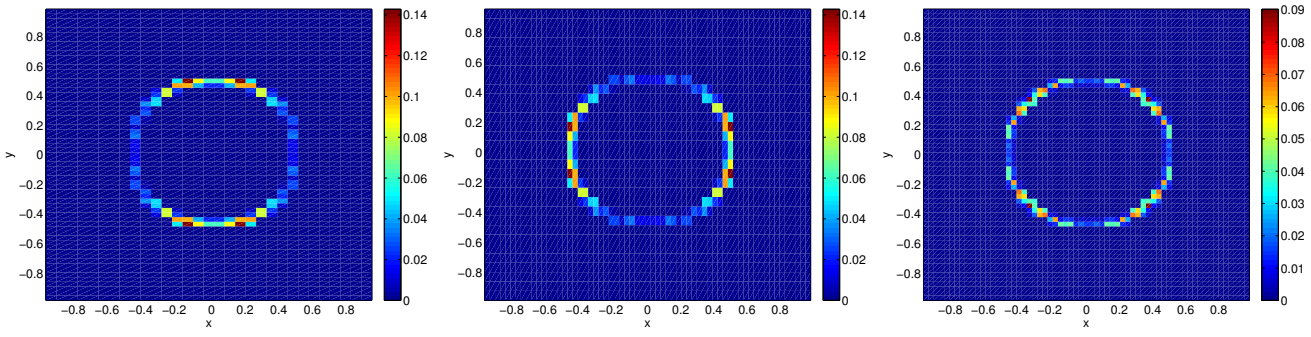
Many areas such as climate modeling, shallow water equations, and computational fluid dynamics use nonlinear hyperbolic partial differential equations to describe the behaviour of some unknown quantity. In general, the solutions of these equations contain shocks, or develop discontinuities. To efficiently apply the discontinuous Galerkin (DG) method in case of discontinuous solutions, an accurate shock detector is needed, in order to determine where the use of a limiter, or adding viscosity is necessary.

In this presentation we discuss the use of multiwavelets for shock detection. We explain how DG coefficients can easily be used for a multiwavelet decomposition of the approximation, [1]. This decomposition is written as a sum of a global average and finer details on different levels. Using such a decomposition allows the multiwavelet expansion to act as a shock detector, where the averages of this contribution are computed on each element, [2]. This allows for shock detection in two-dimensions as well. For example, in two-dimensions, the multiwavelet decomposition uses combinations of scaling functions and multiwavelets in the $x-$, and $y-$direction. This is the reason why we are able to detect the exact locations of discontinuities in the $x-$, or $y-$direction, or in one of the diagonal directions (Figure 1). This is joint work with Jennifer Ryan (University of East Anglia).



(a) Detects $y-$directed shocks (b) Detects $x-$directed shocks (c) Detects diagonal directed shocks

Figure 1: Multiwavelet averages of circle wave, using DG basis polynomials of degree $k = 3$, mesh 64×64.

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Recent Progress Towards Periodic Solutions of the Euler Equations

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I will report on recent progress Blake Temple and I have made towards proving the existence of time-periodic shock-free solutions of the compressible Euler equations. I shall briefly recall our previous results and the main remaining issues in getting the Nash-Moser method to converge. I shall then present details of our approach, which reduces the problem to that of obtaining estimates on finite dimensional projections of linearized operators. The operator can be described in detail, and in principle reduces to the calculation of the smallest singular value of an $N \times N$ matrix.

Industrial Mathematics (SS-IM)

Organizer:
Sean Bohun (University of Ontario Institute of Technology)

Perhaps one of the simplest definitions of Industrial Mathematics as being problem driven mathematics for the sake of science rather while pure mathematics may be regarded as mathematics for its own sake. The term industry is meant in a very broad sense consisting of any field with either a commercial or societal benefit, whether it be the optimal design of an electric motor, modelling financial options or even classifying mother/child interactions. It is characterized by an underlying philosophy of problem-driven rather than area-led mathematics which often results in the novel use of mathematics to highlight cross disciplinary understanding that would not be possible with more traditional methods. This special session will highlight work across the wide spectrum of industrial mathematics illustrating the collaboration of mathematics, science and industry to provide insight to real life problems.

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Modelling Mass Transfer in a Rotating Disk Reaction Vessel

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Presented is research focussing on the process of mass transfer in a rotating disk apparatus, formulated as a Stefan problem driven by the dynamics of the chemical reactions in the bulk solution. Calcite (calcium carbonate) is chosen as the material undergoing dissolution because of the central role it plays in geological and man-made structures. The wide range in the rates of the various reactions allows for a natural decoupling of the problem into a simplified set of weakly coupled convective-reaction-diffusion equations for the slowly evolving species, connected with a set of algebraic relations for the species that react rapidly. Further simplification is possible by identifying the dominant reaction as determined by the acidity. Numerical solutions of the model are compared to the results of an asymptotic analysis and predicted dissolution rates are contrasted with experimentally obtained results.

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3D Modeling of some industrial processes of steel heat treating[1]

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In this work we present some 3D numerical simulations of the industrial procedure of steel heat treating. These simulations have been carried out with the software package Freefem++ ([3]). The geometry corresponds to a car steering rack (Figure 1).

The heating stage includes the description of the electromagnetic variables, the temperature and the austenite evolution ([1]). At the beginning of the cooling stage, the current is switched off, followed by aquaquenching. During this stage, austenite transforms into martensite along the toothed zone so that ductility is maintained on the rest of the workpiece. The workpiece undergoes certain deformations during both stages and they should be taken into account in a complete model ([2, 4]).

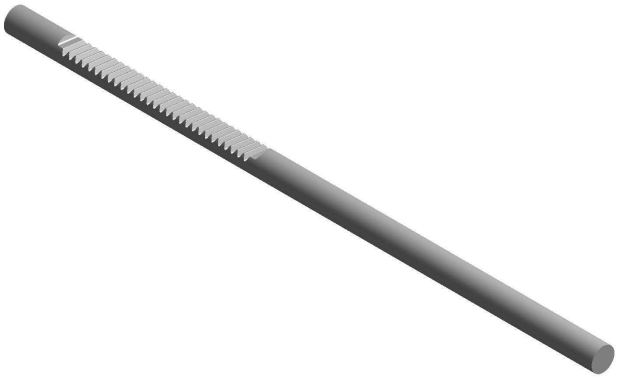

Figure 1: Steering rack of a car showing the toothed zone.

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Optimal Flu Vaccination in a Multiple Group Model

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Flu epidemics occur annually and are frequently a cause for concern. Vaccine is distributed yearly in an effort to reduce the flu's effect, but it is not always clear who should be vaccinated first. We investigate an optimal control problem associated with the administering of vaccine to different groups of people. It is found that optimal solutions take the form of "Bang-Bang" and an appropriate numerical scheme for finding them is thus developed. Using data from a hospital, parameter values for a multiple group SIR epidemic model are found. Then, using the parameter values found from the data, the numerical scheme is implemented to determine optimal vaccination strategies for a population grouped by age. The results are analyzed to see how sensitive they are on the parameters found. The vaccination strategies are also examined to see how they might change given different objectives.

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Modelling and Simulation of Atmospheric Pollutant Dispersion

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Atmospheric dispersion refers to the transport of contaminants in the air under the influence of advection (due to the wind) and turbulent eddy diffusion. The advection-diffusion equation is a parabolic partial differential equation that is most commonly used to model such dispersion problems. When a contaminant is emitted from a stationary point source in a unidirectional wind, then the governing equations admit an analytical solution known as the "Gaussian plume". This plume solution has been exploited by environmental engineers for decades in solving practical emissions problems, and it forms the basis of many efficient and robust software packages for estimating contaminant concentrations under the assumption that the emission rates are known *a priori*. Airborne contaminants arise in a wide range of applications including particles emitted from industrial operations, living organisms (insect swarms, seeds, pollen), natural emissions (volcanic ejecta, smoke from forest fires), and biological agents (radioactive fall-out, infectious microbes).

Our work focuses on the corresponding inverse problem, in which we aim to estimate the source emission rates based on ground-level contaminant measurements. We describe a least squares optimization approach for source estimation [3], and illustrate the approach using an actual study of a zinc smelting operation in British Columbia in which we estimate zinc emission rates for multiple sources that are distributed across the smelter site.

In order to validate our solution to the inverse problem, we also develop a finite volume algorithm for solving the three-dimensional advection-diffusion equation. We apply a fractional-step approach in which the advection terms are integrated first using the high resolution wave propagation method of LeVeque [1], and the diffusion terms are handled using an alternating-direction-implicit (ADI) method [2]. The results are compared with the solution of the inverse problem and conclusions are drawn regarding the accuracy and robustness of our inverse source estimation algorithm. We pay particular attention to the issues of parameter sensitivity and well-posedness of the inverse problem.

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Some recent mathematics-in-industry study group projects from Australia and New Zealand

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Since 1984 Mathematics in Industry Study Groups have been held in Australia and New Zealand [1]. I have participated in these annual week-long meetings since 2004. In this talk I will review some of the kinds of projects that have been brought to these meetings and particular ones that I have worked upon. Among the industries involved are those of steel manufacture, electricity transmission and agriculture, e.g. [2, 3, 4].

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Quality assessment of medical images using the structural similarity index

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Given the explosive growth of digital image data being generated worldwide, medical communities have recognized the need for increasingly efficient methods of storage, display and transmission of medical images which, in turn, will necessitate improved compression techniques as well as reliable quality assessment methods. Our study, involving a collaboration with radiologists (DK,NSK) as well as a leading international developer of medical imaging software (AGFA), is primarily concerned with improved methods of assessing the diagnostic quality of compressed medical images and the investigation of compression artifacts resulting from JPEG and JPEG2000. The radiological community has not yet accepted a single objective assessment method for the quality of medical images. Recommended compression ratios for various modalities and anatomical regions have been published [1, 2]. To date, these recommendations have been based on experiments in which radiologists subjectively assess the diagnostic quality of compressed images. On the other hand, the "quality" of a compressed image can be characterized objectively in several ways. Radiologists most often employ the mean squared error (MSE) and its close relative, PSNR, even though they are known to correspond poorly to visual quality. The failure of the MSE is partially due to the fact that spatial relationships are ignored by the L^2 metric [3]. A more recent image fidelity measure, the SSIM index [4], measures the difference/similarity between two images by combining three components of the human visual system - luminance, contrast and structure. The result is a much improved assessment of visual quality. In this work, we compare the performances of SSIM, MSE/PSNR, compression ratio C_R and JPEG quality factor Q, based on experimental data collected in two experiments involving radiologists.
The first experiment involved a global quality assessment of 100 brain and body CT images at various compression ratios. The radiologists evaluated compressed images as acceptable or unacceptable as compared to their uncompressed counterparts. An ROC and Kolmogorow-Smirnov analysis indicates that compression ratio is not always a good indicator of visual quality. Moreover, SSIM demonstrates the best performance, i.e., it provides the closest match to the radiologists' assessments. We also show that a weighted Youden index and curve fitting method can provide SSIM and MSE thresholds for acceptable compression ratios. The second experiment involved a local/regional image quality analysis of these images by the radiologists. An ROC analysis once again shows that SSIM provides a closer match to subjective assessments.

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Lie Symmetry and Other Approaches in Theory and Applications of Nonlinear Equations (SS-LSNE)

Organizers:
C.M. Khalique (North-West University)
M. Abudiab (Texas A&M University)

This session is devoted to all research areas that are related to nonlinear differential equations and their applications in science and engineering. The main focus of this special session is on the Lie symmetry analysis and its applications to ordinary and partial differential equations. Other approaches in finding exact solutions to nonlinear differential equations will also be discussed. This includes, but not limited to, asymptotic analysis methodologies, the simplest equation method, the (G'/G) expansion method, inverse scattering transform techniques, the upper-lower solutions method, the Hirota method, the Adomian decomposition method, and others.

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Exact solutions of a (3 + 1)-dimensional B-type Kadomtsev-Petviashvili equation

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A (3+1)-dimensional generalized B-type Kadomtsev-Petviashvili (BKP) equation will be examined.This equation is an extension of the well-known Kadomtsev-Petviashvili equation, which describes weakly dispersive and small amplitude waves propagating in a quasi-two-dimensional media. The simplest equation method will be used to construct exact solutions of this B-type Kadomtsev-Petviashvili equation.

[1] presenter

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Symmetry analysis and exact solutions of semilinear Schrodinger equations

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Semilinear Schrodinger equations provide a model of many interesting types of nonlinear waves, e.g. laser beams in nonlinear media, plasma waves, free surface water waves. This talk will apply a novel symmetry method [1, 2, 3] to find exact solutions for Schrodinger equations with a power nonlinearity in multi-dimensions. Many explicit new solutions are obtained which have interesting analytical behavior connected with blow-up and dispersion. These solutions include new similarity solutions and other new group-invariant solutions, as well as new solutions that are not invariant under any symmetries of the Schrodinger equation. In contrast, standard symmetry reduction methods lead to nonlinear ODEs for which few if any explicit solutions can be derived by familiar integration methods.

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A Note on Wavelet Approximation Techniques for Differential Equations

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In this study we have presented wavelet approximation techniques for differential equations in a detailed manner. We have discussed what the advantages and disadvantages of wavelet basis are when they are used in the solution of ODE's and PDE's some boundary and initial conditions.

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Symmetry reductions and exact solutions of a generalized Fisher equation

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In this paper, we study a generalized Fisher equation by using the theory of symmetry reductions in partial differential equations. Optimal systems and reduced equations are obtained. We derive some traveling wave solutions by applying the $\frac{G'}{G}$-expansion method. Among these solutions we get solutions which describe kinks, solitons and periodic solutions.

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Lie group classification for a generalized coupled Lane-Emden system of dimension one

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In this talk we study the generalized coupled Lane-Emden system $u'' + H(v) = 0$, $v'' + G(u) = 0$, which has many applications in several physical phenomena. We carry out the complete Lie group classification of the underlying system. We show that the system admits a ten-dimensional equivalence Lie algebra. It is also shown that the principal Lie algebra, which in one dimensional, has several possible extensions.

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Solutions of the Klein-Gordon-Zakharov equations using simplest equation method

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In this talk we look for exact solutions of the Klein-Gordon-Zakharov (KGZ) equations, which describes the interaction between Langmuir waves and ion sound waves. The KGZ system consists of coupled equations of two functions $u(x,t)$ and $v(x,t)$, where the function $u(x,t)$ is complex and denotes the fast time scale component of electric field by electrons and the function $v(x,t)$ is real and denotes the deviation of ion density from its equilibrium. The method used to obtain exact solutions will be the simplest equation method. The solutions obtained will be the travelling wave solutions.

[1] presenter

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Exact solutions to two coupled nonlinear evolution equations

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In this talk we obtain exact solutions of two nonlinear coupled evolution equations. These nonlinear coupled equations appear in a variety of science and engineering applications such as fluid dynamics, plasma physics, nonlinear optics, etc. The two nonlinear evolution equations are the coupled Kortweg de Vries equations

$$\begin{aligned} u_t + 6uu_x - 6vv_x + u_{xxx} &= 0, \\ v_t + 3uv_x + v_{xxx} &= 0 \end{aligned}$$

and the coupled Boussinesq equations

$$\begin{aligned} u_t + uu_x + v_x + \alpha u_{xxt} &= 0, \\ v_t + (uv)_x + \beta u_{xxx} &= 0. \end{aligned}$$

We employ the $(G'/G)-$expansion method to seek exact solutions of the underlying systems.

[1] presenter

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Conservation laws of a system of coupled KdV equations

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The modeling of several physical phenomena such as, the interaction of two long waves, whose dispersions relations are different, give rise to the coupled Korteweg de Vries system. In this talk we derive the conservation laws of the coupled Korteweg de Vries system by using some transformations and then invoking Noether's theorem.

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Particles control in fragmentation equations

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Fragmentation processes can be observed in natural sciences and engineering. To provide just a few examples, we mention the study of stellar fragments in astrophysics, rock fracture, degradation of large polymer chains, DNA fragmentation, evolution of phytoplankton aggregates, liquid droplet breakup or breakup of solid drugs in organisms [1, 2, 3]. Fragmentation processes are difficult to analyze as they involve the evolution of two intertwined quantities: the mass of the ensemble and the number of particles in it. That is why, though linear, they display nonlinear features such as phase transition which, in this case, is called shattering and consists of a formation of 'dust' particles of zero size, but, nevertheless, carrying a non-zero mass. To investigate these phenomena, we consider the fragmentation equation in the space of densities yielding both a finite number of particles and a finite mass of the ensemble. We derive an analytic expression for the resolvent of the governing integro-differential equation and make use of it to examine the spectral properties of the fragmentation operator. Furthermore we use Arendt-Robinson-Batty theorem to prove that the fragmentation operator generates a strongly continuous semigroup in the given space. In particular, we show that in some shattering fragmentation processes, one can typically control the total number of particles in the system.

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Power geometry for a reversible system of ordinary differential equations

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We consider reversible system of ODEs fourth order depending on two small parameters $X'' = (x_5, x_6)$:

$$\dot{X}' = \Phi(X', X''), \quad X' \in R^4, \quad \dot{X}'' = 0, \quad X'' \in R^2. \tag{1}$$

Here $X = (X', X'')$, $X' = (x_1, x_2, x_3, x_4)$, where $\Phi(0, X") = 0$, and the point $X' = 0$ is stationary, and the matrix of the unperturbed linear part L in $X = 0$ is a Jordan block with four-fold zero eigenvalue. Also it is supposed, system (1) is invariant under the substitution $X', X'', t \to SX', X'', -t$, where $SX' = (x_1, -x_2, x_3, -x_4)$, i.e. the property of reversibility of system (1) means that

$$S\Phi(X', X'') = -\Phi(SX', X''). \tag{2}$$

Such a system appears in Hydrodynamics. For example, the problem of surface water waves for the Bond number b close to $1/3$ and the Froude number $\widetilde{\lambda}$ close to 1 is transformed into system (1) as a result of reduction on the center manifold (see [3]).

The solutions to the system (1) are studied in the neighborhood of the stationary point $X = 0$ in the following way. The linear part of system (1), which depends on parameters, is reduced to the normal form. The lower triangular matrix of parameters is obtained, in such a way that each its diagonal consists of equal parameters. In the second diagonal from below and in the main diagonal there are only zeros because of the property (2). We discover the support $D \in R^6$ of system (1), i.e. the set of power exponents and using it we computed Newton polyhedron in R^6 by the program (see [1-2]). With the table of correspondence we extract all the set of truncated systems. We obtained only five truncated systems of maximal "dimension" five. Among them there is the basic truncated system which after the power transformation (see [1-2]) which the number of parameters is reduced to one and this system is reduced to the system

$$\dot{y}_1 = y_2, \quad \dot{y}_2 = \sigma y_1 + y_3, \quad \dot{y}_3 = \sigma y_2 + y_4, \quad \dot{y}_4 = \nu y_1 + \sigma y_3 + a y_1^2, \tag{3}$$

where $\sigma = \pm 1$,parameters ν and $a \in R$. It is shown that system (3) is a Hamiltonian one and it has only two independent quadratic first integrals. The main result of this work is the existence of new families of periodic waves and of new families of quasi-periodic waves for $\nu < 0$, which we have received.

Here we demonstrated the effectiveness of methods of Power Geometry (see [1,4]) for the investigation of rather complicated singularities on the example of system (1). We tried to use as simple algorithms of computations as possible, which allowed us to complete computations to the end.

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A Computational Study of Forced Oscillations of a Korteweg-de Vries Type Equation

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We will present a solution to a Korteweg-de Vries (KdV) type equation with periodic boundary conditions. It has been observed experimentally and shown theoretically that the solutions to this system eventually become periodic, with the same period as the forcing at the boundary, and we demonstrate these results with an efficient numerical algorithm. A collocation method is used to solve the initial and boundary value problem of KdV equation.

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Modeling Approaches and Challenges in the Build Enviroment (SS-MACBE)

Organizers:
Ryan Danks (RWDI)
Michael Carl (RWDI)

As urban densities increase, understanding the interactions between climate, the built environment, and the local population are increasingly important subjects. Energy efficiency, minimizing heat island effects and general satisfaction of the inhabitants are becoming driving forces in modern sustainable design. The urban landscape is a complex system where wind, solar radiation and other climatological parameters impact everything from building energy usage, building structural requirements and pollutant dispersion to thermal comfort and the creation of pleasant environments. In this session, some of the methods and approaches used in studying a variety of issues within cities and around buildings will be presented.

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Analytical study of wave run-up generated by bottom motion on a non-uniformly sloping beach

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Tsunami is known for its characteristic run-up heights which makes it significantly different from the other wind generated waves [1, 2, 3]. Although researchers are quite in agreement that bottom topography of ocean plays an important role in determining run-up [4], even the recent two field studies [5] & [6] also suggest that, still in an analytical study of the problem there seems to have been no attempt to include variability of bottom topography. The inclusion of variable bottom topography makes the underlying hydrodynamic problem critical, which is perhaps one of the reasons of avoiding this factor. In our attempt we have tried to provide an analytical solution of the problem of generation of tsunami waves by an instantaneous arbitrary ground motion in an ocean with a variable slope. We used linear shallow water equation [1] for a beach with variable slope $y = -qx^r$ and $q > 0,\ r > 0$, referred to horizontal and vertical directions as x- and y-axis respectively and presented an analytical expression of run-up. The effect of bottom topography on the run-up is discussed. In the process of our analysis, several other results in regard to wave behaviour has come up which are interesting in their own rights particularly in comparison to those obtained with the constant slope beaches.

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Energy Use Analysis at the Master Plan Level

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In the early stages of master plan design, street layouts, zoning, building materials and building shape/orientation are in flux. These design decisions have both a capital and energy use cost, making an understanding of their relative effect on energy use important in master plan development. However, generating preliminary energy use estimates can be difficult. This is because traditional methods of estimating energy use with energy modeling software and tools are overly detailed, time consuming and require significant assumptions about the design. To meet this need RWDI developed the Master Plan Energy Profile (MPEP) Tool.

The MPEP offers a compromise between simplifications at the building level and speed/ease of completing design analysis. The MPEP tool can rapidly calculate energy demand based on solar loading/shading (from adjacent buildings), heat transfer through windows and walls using local climate data and space usage type and scheduling (occupancy, lighting etc.). The tool completes its rapid calculations based on the buildings perimeter and gross flow area and building information inputted by the user. Therefore, the tool is best used for comparative analysis and value engineering rather than detailed energy use predictions of the master plan. The comparative analysis can be performed on design decisions with respect to window to wall ratio (WWR), glazing type and construction, wall insulation values, building orientation and building usage parameters such as lighting power density (LPD). It can also be used to estimate the impact of renewables and other building integrated energy saving technologies.

A MPEP model is constructed by first simplifying the building geometry into block shapes and defining these blocks in the tool using the user interface or a spreadsheet input file. Building usage and construction details are then entered as well as location and weather information. Building construction and usage information is typically estimated by the design team or values from guidelines such as those from the American Society of Heating and Air-Conditioning Engineers (ASHRAE). Once a baseline energy demand has been established, areas of high energy demand can be identified and conservation measures implemented in order to reduce energy use. When implementing conservation measures, changes can be made at the individual building or groups of building level. Calculating the results takes on the order of minutes allowing for many scenarios to be run and reported quickly. The tool provides value in allowing designers to see the "big dial" sensitivity of their development and inform financial decisions such as should money be spend on improving windows or re-orienting the buildings.

RWDI has used the tool on many projects around the world in diverse climates such as China and the Middle East.

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Large Scale Modelling of Human Thermal Comfort in the Urban Realm

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As modern architects and master planners strive to create walkable, pedestrian friendly environments within the urban realm, more emphasis is being placed on ensuring that such spaces are as comfortable as possible, as often as possible. In some juristictions [1] pedestrian comfort is even codified as part of green building standards. Thus, shifting the view of outdoor thermal comfort from an afterthought to a factor that directly impacts the design process.

Estimating thermal comfort outdoors is a complex problem, requiring knowledge of historic climate patterns, local wind and solar conditions, as well as human physiology and psychology. Local conditions, such as a particular street corner or outdoor café are challanging to assertain as they will vary both in space and time, nessecitating a high degree of resolution. These challenges are compounded by the ever increasing scale and complexity of architectural designs, and ever decreasing time-lines for such work in industry.

Improving upon previous methodologies developed at RWDI [2], the approach outlined here allows thermal comfort analyses to be conducted over hundreds of hecatres at metre-scale resolutions, while better simulating the effects of semi-transparent obstructions (e.g., trees, canopies) as well as diffuse radiation eminating from the sky. Moreover, this method is easily scaleable allowing larger domains to be processed quickly by leveraging RWDI's own computing cluster, or other cloud based high performance computing services.

RWDI's *ThermalComfort360* approach first involves a meteorlogical analysis based on either locally measured climate data or data extracted from meso-scale Weather Research and Forcasting (WRF) models. Based on this data, the prodominant wind directions at the site are selected for simulation using the computational fluid dynamics (CFD) package, OpenFOAM. These simulations include all significant surrounding buidlings and topological features and quantify the effects they have on the local wind microclimate.

The second step leverages a custom solar analysis engine, built on the open-source framework of OpenFOAM, which allows total solar insolation to be computed at each point in the computational domain. The native parallelization of the OpenFOAM libraries and the ability to leverage the existing computational grid from the CFD study provide significant advantages in both speed and resolution of such studies and the open source nature of the code allows for on-going improvement to the methodology and the abilty to generate non standard outputs quickly and efficiently. This engine iterates through the extracted climate data, which is typically at least one year of hourly records, calculating solar levels, wind conditions based on the existing CFD analyses, and finally outputing a number of thermal comfort metrics.

The results are then presented as coloured contour plots at pedestrian level to highlight any areas of concern to the client and assisting in the planning of any mitigative measures.

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Applicability of a Diffusion Model for Cosmic Ray Transport during Large Forbush Decrease Events

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A collection of physical processes beginning at the Sun and ultimately affecting human activities on Earth and in space is described by the term 'Space Weather' (SW). When a Coronal Mass Ejection (CME) is erupted from the Sun and, travelling in space, reaches Earth it can cause a SW phenomenon called a geomagnetic storm which has severe impacts on critical infrastructures. Such effects can disrupt communications from satellites and produce geomagnetically induced currents in power systems. They also affect the cosmic radiation environment and change the radiation dose for aircrew on polar flights. One of the tools which can serve as a useful source of information for SW monitoring and forecasting is ground-based cosmic ray (CR) detectors.

CRs often experience a rapid decrease in intensity associated with CMEs, which is called Forbush Decrease (FD). One of the mechanisms providing FD effect is assumed to be diffusion of CRs on fluctuations of the Interplanetary Magnetic Field (IMF) produced by CMEs. To estimate a diffusion coefficient, the IMF power spectrum is used. To analyze the spectrum, IMF-spectrograms produced by use of satellite data are employed. To improve resolution of spectrogram in both time and frequency, a special procedure of averaging over spectrograms with different window lengths is applied. Based on the obtained IMF spectrograms the validity of the diffusion model for CR transport during large FD events is verified.

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A Cantor Set Model of Earthquake Dynamics in Aftershock Sequences

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The origin of earthquakes is assumed to be based on the theory of faulting. Earthquake dynamics is the study of the interactions of two opposing fault surfaces which produce seismic activity. Over the last five decades, a number of models have been proposed that try to simulate seismic activity by mimicking the interlocking of opposing rock surfaces. The validity of a given model is subject to the compliance of the synthetic seismic activity it produces to well known empirical laws which describe the statistical features of observed seismic activity. The overall frequency distribution of earthquakes is given by the Gutenberg-Richter (GR) Law which states

$$\log N(m) = a - bm \tag{1}$$

where *N(m)* is the frequency of earthquakes with magnitude greater than or equal to *m* occurring in a specified area, *a* and *b* are constants. Secondly, the temporal distribution of aftershocks of magnitude *m* greater than some threshold value M_c is given empirically by the Omori Law,

$$\frac{dN(t)}{dt} = \frac{1}{t^p}, \qquad m > M_c \tag{2}$$

where *dN(t)/dt* gives the rate of occurrence of aftershocks at time t after the the main earthquake.

We introduce a purely geometric model of earthquake dynamics using Cantor sets (Fig. 1). The model tries to emulate the stick-slip dynamics of fractal surfaces by evaluating the time-evolution of overlap lengths of two identical Cantor sets sliding over each other. We demonstrate that the statistical aspects of aftershock sequences are naturally captured by this simple model.

More importantly, this model also reveals a new statistical feature of aftershock sequences which we have verified to be present in nature as well. We show that, both in the model as well as in nature, the cumulative integral of aftershock magnitudes over time is a remarkable straight line with a characteristic slope. This slope is closely related to the fractal geometry of the fault surface that produces most of the aftershocks. We also discuss the implications that this feature may have in possible predictions of aftershock magnitudes or times of occurrence.

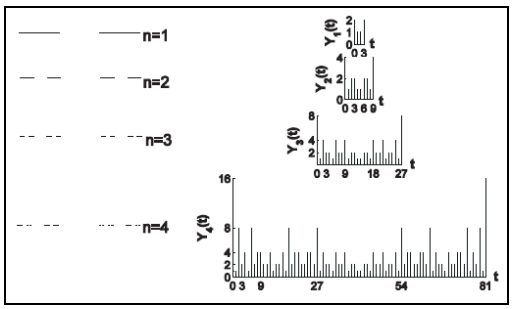

Figure1: The recursive structure of the time series for the first four generations in thefractal-fractal overlap model. On the left the respective Cantor set generations are shown. Noticeable is the fact that the time series of all preceding generations are embedded within the time series at a given generation.

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Computational Methods and Applications in Building Ventilation

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Ventilation is an important aspect of building design, and has significant impact on occupant comfort, health, and safety. Sufficient ventilation can be achieved by forced means, such as air handling units, jet fans, etc., or by natural means, such as wind towers, openings in the façade, etc. Building designers often strive to reduce use of forced ventilation to achieve environmental goals and savings on operating costs.

To help inform this design process, Computational Fluid Dynamics (CFD) as well as wind tunnel testing can be used to gain insight into the exterior wind flow and its influence on interior air flow of a building. An example case is presented for an underground parking garage at a residential development that is partly naturally ventilated to demonstrate the use of these tools. The ventilation system is proposed and optimized for both normal and emergency modes of operation. The goal of normal mode ventilation is to provide sufficient exhaust of vehicle emissions to maintain acceptable carbon monoxide (CO) concentrations everywhere in the garage, while the goal of emergency mode ventilation is to provide sufficient exhaust of smoke to allow safe egress of occupants. Overall, the design team is interested in energy conservation and lowering operating costs, so natural ventilation is also incorporated into the design.

Wind tunnel testing is used to help understand the wind flow patterns at the building site. Multiple highrise condominiums are planned for above grade, which is expected to affect the local wind flow. A scale model of the buildings above grade as well as surroundings is constructed and tested in the wind tunnel for a range of wind conditions. The wind pressure data is used to help determine the location, direction and number of wind towers. CFD modelling is used to help optimize the wind tower inlet shape. A constant volume thermodynamic analysis combined with wind pressure data and site meteorological record is performed to assess the energy savings potential of the wind tower arrangement.

The spread of vehicle emissions and smoke are simulated using CFD. The incompressible Navier-Stokes equations of fluid flow, coupled with transport equations for energy, CO and soot, are discretized using the finite volume method. Appropriate source terms are included when appropriate, such as gravity/buoyancy, and volumetric generation of soot and heat for fire modelling. Turbulence is modelled using Reynolds averaging with realizable k-epsilon turbulence closure. The equations are solved subject to boundary conditions for supply air and exhaust, the influence of wind towers, as well as CO emissions. A commercial CFD software, CD-adapco's STAR-CCM+, is used and the equations are solved using its standard segregated solver (SIMPLE algorithm), where the equations are iterated one by one using an algebraic multigrid approach.

The results of the CFD analysis are used to optimize the garage layout and ventilation system design, and to satisfy relevant regulatory requirements, such as building codes, fire codes, etc.

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Numerical Weather and Climate Prediction for Building Science

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Representative meteorological and climatological information are crucial to many aspects of building science. However, in many parts of the world, sparse measurement monitoring networks and/or complex topography result in a paucity of site specific meteorological data suitable for these studies. In such situation applications of prognostic meteorological model permits engineers to develop simulated site specific meteorological and climatological information to replace measurements from nearby monitors. In addition, because the model provides a three-dimensional simulation of atmospheric processes, the model results may be used to investigate vertical distribution of meteorological parameters more accurately that can be obtained by using standard methods to extrapolate surface based measurements upward. Further, as the prognostic models incorporate the influence of land surface characteristics on atmospheric processes, they may be used to estimate future meteorological and climatological response to anthropogenic changes in the earth surface, such as urban growth.

In recent years, RWDI has employed the Weather Research and Forecast Model (WRF) to provide meteorological modeling for numerous studies in varied setting around the world. WRF is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict atmospheric circulation on scales ranging from 100's of meters through to 1000's of kilometers. WRF allows the ability to conduct simulations reflecting either real data or idealized configurations. The effort to develop WRF has been a collaborative partnership, principally among the NCAR, the National Oceanic and Atmospheric Administration (NOAA), the National Centers for Environmental Prediction (NCEP), the Forecast Systems Laboratory (FSL), the Air Force Weather Agency (AFWA), the Naval Research Laboratory, the University of Oklahoma, and the Federal Aviation Administration (FAA).

Several case studies showing the development and application of simulated weather information for building science will be presented.

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Minimum Stack Height for Micro Aerosols Air Pollution

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This work deals with air pollution management for stationary sources micro aerosols obtained from the industrial stacks in the box areas atmosphere. The most widely used Gaussian model that is the core of almost all regulatory dispersion models is used to explain the distribution of the plume. Question is to manage the minimum height for the existed stacks such that one does not exceed the legal thresholds on pollution emissions. Mathematical formulation of this problem yields to the specific semi-infinite programming. Novel Numerical optimization technique based on discretization method is proposed successfully. The optimal height for the stacks is calculated for the work example problem and it is shown that the current method computes the minimum heights better than the existed models.

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Modeling Building Stack Effect Using Network Model

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As the world becomes more urbanized, interactions between various elements in and around buildings are increasingly complex. Numerical modeling is often desirable to analyze potential building-related issues such as energy use, safety and comfort. This talk focuses on one aspect of the interactions between a building and its environment – the stack effect phenomenon.

Stack effect in a building occurs when there is a temperature difference between indoor and outdoor. During winter time in cold climate, the conditioned environment within the building is much warmer than the exterior environment. Ideal gas law infers that the indoor air density is lower than the exterior air density under similar pressure condition. Since both the building and its environment are under the influence of gravity, the difference in density leads to a difference in hydrostatic pressure. During winter time in cold climate, the resulting pressure differences act to push air out of the building near the top of the building and bring exterior air into the building near the base. This phenonmenon is termed stack effect. The total hydrostatic pressure difference for a buiding of height H conditioned to temperature T_i with an outdoor temperature of T_o can be approximated by the following simplified equation:

$$\Delta P = gH\rho_i\left(1-\frac{T_i}{T_o}\right) \tag{1}$$

where g is the gravitational acceleration; ρ_i is indoor air density. As inferred in the equation, the potential for issues is greatest for tall buildings in cold climate.

Since the pressure difference created by stack effect phenomenon acts on the entire exterior surface of the building, numerical analysis needs to include the entire building volume in order to deduce the summary effect of all elements in the building. Dynamics of flow within an entire building is typically modeled using a network model. In the network model, nodes represent continuous spaces such as rooms, corridors and outdoors while links represent the dividing elements such as walls and doors. The inherent assumption in the model is that the physical properties in each of the continous spaces are constant throughout. This simplification is possible because the resistances to flux of physical properties are orders of magnitudes larger through the dividing elements than within the continuous spaces.

By applying network model to the a building, many potential issues in client projects can be highlighted and mitigated. These include cold drafts in winter, excessive energy loss, difficulty opening doors and constant whilstling through doors.

Modeling and Computational Methods for Mathematical Biology and Medicine (SS-MCMMBM)

Organizers:
Suzanne Shontz (Mississippi State University)
Corina Drapaca (The Pennsylvania State University)
Siv Sivaloganathan (University of Waterloo)

Today, mathematical modeling and computational methods and simulations play essential roles in the advancement of biomedical sciences, providing us with a better understanding of biological systems and disease patterns and ultimately contributing to the fast development of modern prevention, diagnostic and therapies tools needed by the medicine of tomorrow. The aim of this session is to bring together mathematicians, physicists, engineers, and clinicians involved in the area of biomedical sciences to provide state-of-the-art reviews, and report on current cutting-edge research and open problems. It is hoped that bringing together researchers with such a wide range of expertise will create the right environment for idea dissemination and fruitful discussions.

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Myelosuppression and cytokine interaction in a mathematical model of the human hematopoietic system

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The production of human blood cells is regulated through a highly complex, coupled set of feedback mechanisms involving, among others, differentiation of cell lines from a common pool of stem cells and hormonal interactions between circulating cells and cells at different stages of maturation. As part of a global modeling project of the full hematopoietic system, we investigate possible pharmaceutical interventions using a structured model for the 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 control mechanisms relating the circulating cells to the maturation process: some of the delays are therefore state-dependent.

Concentrating on the regulation of neutrophils, we analyse the perturbative effects of different chemotherapeutic regimens on equilibrium solutions and their destabilisation by Hopf and secondary bifurcations. We obtain dynamical interpretations for the neutropenic episodes, as well as conditions for the simultaneous stability of multiple equilibria: the influence of scheduling, as well as the remedial use of G-CSF, is particularly emphasized. Parameter estimation and compatibility of the behavior of the solutions of our model with clinical practice will be discussed.

Joint work with Michael C. Mackey, Tony Humphries, Grace Brooks and Gabriel Provencher-Langlois from McGill University, Morgan Craig, Jun Li and Fahima Nekka from Université de Montréal, and Jinzhi Lei from Tsinghua University.

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Cluster Newton Method for Sampling Multiple Solutions of an Underdetermined Inverse Problem: Parameter Identification for Pharmacokinetics

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A new algorithm is proposed for simultaneously finding multiple solutions of an underdetermined inverse problem. The algorithm was developed for an ODE parameter identification problem in pharmacokinetics for which multiple solutions are of interest. The algorithm proceeds by computing a cluster of solutions simultaneously, and is more efficient and more robust than existing algorithms because it fits the Jacobian in a collective way using a least squares approach. It is demonstrated numerically that the algorithm finds accurate solutions that are suitably distributed, guided by a priori information on which part of the solution manifold is of interest, and that it does so more efficiently than standard methods. It is also demonstrated that the algorithm is more robust against noise in the function evaluations than standard methods.

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A Study of Brain Biomechanics using Hamilton's Principle

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Most of the current research in brain biomechanics is focused on how best to relate continuum mechanics and stress-strain constitutive laws to the biochemistry of the evolving microstructure of brain. The luck of experimental data needed by these models and the complexity of the required computations make these models useless in clinical applications for now. To capture some of the dynamics taking place at different scales during the evolution of neurological diseases and are as simple as possible we propose a couple-field model using Hamilton's principle. For a 1D model of the brain, we assume that the mechanical response of the brain tissue at the macroscopic level is linear visco-elastic of Kelvin-Voight type. The 1D brain tissue of mass density m, effective elastic modulus $\bar{E}$, length L and constant area A has one fixed boundary ($x=0$) at the interface with the meninges and one moving boundary ($x=L$) at the interface with the ventricular cerebrospinal fluid which undergoes macroscopic displacements $u(x,t)$ caused by the heart pulsations and aging. We also assume: 1) a microstructural healthy growth (or healing) of brain with $\phi_g(x,t)$ the current growth state, and 2) a microstructural inflammation of the aging brain that progresses slowly throughout the lifespan [1] with $\phi_i(x,t)$ the current inflammation state. Inspired by [2], we define the Lagrangian as: $\mathscr{L}=\int_0^L\left[\frac{1}{2}m\dot{u}^2+\frac{1}{2}m\alpha(\dot{\phi_g}^2+\dot{\phi_i}^2)-\frac{1}{2}\bar{E}(\phi_g,\phi_i)Au'^2-\frac{1}{2}\beta(\phi_g'^2+\phi_i'^2)\right]dx,\ \alpha,\beta>0$, with $\dot{u}=\partial u/\partial t$, $u'=\partial u/\partial x=J-1$, J the Jacobian of the deformation, and let the virtual work be: $\delta\mathscr{W}=\int_0^L\left[f\delta u-c\dot{u}'\delta u'-\Phi_g(\phi_g,\phi_g',\dot{\phi_g})\delta\phi_g-\Phi_i(\phi_i,\phi_i',\dot{\phi_i})\delta\phi_i\right]dx+F\delta u|_L$. By applying Hamilton's principle, taking $\bar{E}=\lambda\phi_g(1-\phi_i)$ and making some simplifications we get: $\ddot{\phi_g}=-(J-1)^2(1-\phi_i)$, $\ddot{\phi_i}=(J-1)^2\phi_g$ which we solve using the volumetric data from [3] for healthy and hydrocephalic mice. For initial conditions $[\phi_g,\phi_i,\dot{\phi_g},\dot{\phi_i}]=[1,0,0,2.2204e-016]$ we see the expected increase of inflammation and healing decrease in aging normals (Fig.1a), and a competition between the healing and inflammation states in untreated hydrocephalus (Fig.1b).

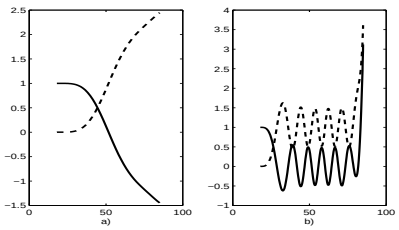

Figure 1: Growth (solid) and inflammation (dashed) states versus time (in days) for a) normal and b) hydrocephalic mice.

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Calcium dynamics in dendritic spines: A link to structural plasticity

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Calcium signals evoked either by action potential or by synaptic activity play a crucial role for the synaptic plasticity within an individual spine. Because of the small size of spine and the indicators commonly used to measure spine calcium activity, calcium function can be severely disrupted. Therefore, it is very difficult to explain the exact relationship between spine geometry and spine calcium dynamics. Recently, it has been suggested that the medium range of calcium which induces long term potentiation leads to the structural stability stage of spines, while very low or very high amount of calcium leads to the long term depression stage which results in shortening and eventually pruning of spines. Here we propose a physiologically realistic computational model to examine the role of calcium and the mechanisms that govern its regulation in the spine morphology. Calcium enters into spine head through NMDA and AMPA channels and is regulated by internal stores. Contribution of this calcium in the induction of long term potentiation and long term depression is also discussed. Further it has also been predicted that the presence of internal stores depletes the total calcium accumulation in cytosol which is in agreement with the recent experimental and theoretical studies.

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Modeling Cell-Sheets Wound Closure

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In the present study, we consider a particular yet major aspect of wound healing, namely the one related to the movement of wounded epithelial cell monolayers. The epithelial monolayer cell population, also referred to as cell-sheet, can be seen as a 2 dimensional structure, although it is well known that apical and basal sites play distinctive important roles during the migration, as well as the substrate itself. Immediately after a wound is created, the cells start to move in order to fill in the empty space. This movement, the wound closure, is a highly-coordinated collective behavior yielding a structured cohesive front, the wound leading edge. Even though wound closure involves biochemical and biomechanical processes, still far from being well understood, which are distributed over the whole monolayer, much specific attention was paid to the leading edge evolution, seen as the front of a traveling wave of the cell density function.

It is then very tempting to investigate the ability of simple PDEs which exhibit traveling waves behavior to model the leading edge evolution. The most known one is the Fisher and KPP equation (F-KPP). F-KPP equation is a nonlinear parabolic partial differential equation, introduced in 1937 by Fisher and Kolmogoroff-Petrovsky-Piscounoff which models the interaction of Fickian diffusion with logistic-like growth terms.

Let denote by Ω a rectangular domain (typically an image frame of the monolayer), by Γ_D its vertical sides and by Γ_N its horizontal ones. We assume that the monolayer is at confluence, and consider the cells density relatively to the confluent one. The F-KPP equation then reads $\frac{\partial u}{\partial t} = D\Delta u + ru(1-u)$ over Ω, and Dirichlet (resp. Neumann) condition is set over Γ_D (resp. Γ_N). One of the main features of the F-KPP equation is that it drives initial conditions u_0 of compact support (e.g. an initial 1-0 step function) to closure (to the stable steady solution $u = 1$) by propagating the front with a constant velocity $V_{th} = 2\sqrt{rD}$ (up to a short transition time). Maini et al. [1] studied a 1D F-KPP validation, experimental leading edge velocities were assumed to be close to V_{th} and were used to fit the diffusion coefficient D given the proliferation rate r (doubling time tables excerpt from published data).

In our case, we perform a parameter identification of the two parameters (r, D), using a 2D simulation of the F-KPP equation, and advanced image processing to minimize the error between computed and biological observed experimental wound closure.

Conclusion : We show that, for non inhibited wound assays, closure occurs at constant speed of the leading edge, a fact that is commonly shared by biologists and biomathematicians. But we also show that the leading edge may exhibit accelerated profiles, and that when inhibited, then the F-KPP has poor performances in modeling the leading edge dynamics.

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Predicting nonlinearity of tumor spheroid growth in HGF media: a data-driven multi-species continuum model

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The mechanochemical interactions of a growing tumor with its microenvironment are increasingly considered to be critical in promoting growth and spread of the tumor. One mechanism by which such interactions occur is via increased secretion of Hepatocyte Growth Factor (HGF) by cancer-associated stromal cells, which has been shown to promote tumor growth and motility [1]. In order to better understand the quantitative nature of HGF on tumor growth, we develop an experimental system using colon cancer initiating cell (CCIC) spheroids grown in media in varying concentrations of HGF, and use the experimental data alongside appropriate literature to extend a multi-species continuum model of solid tumor growth to include action of HGF [2, 3]. The experimental observations show that the rate of tumor growth is nonlinear with respect to HGF: the rate increases with increasing concentration of HGF to 100ng/ml, but decreases to a lower growth rate at higher HGF concentrations. We incorporate this novel information into the mathematical model and use the numerical solutions to obtain a prediction at which HGF concentration the peak in tumor growth rate occurs. The model shows that (i) the HGF concentration at which the peak growth rate occurs depends on the amount of intratumoral HGF, and (ii) growth rate depends on initial spheroid size, which may explain part of the variability observed in the experimental results. Hence, an integrated mathematical/experimental approach allows us to better quantitatively understand the nature of HGF-induced tumor growth and variability therein, and to develop testable hypotheses for the nonlinear nature by which HGF acts on growing tumors.

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The Mechanism Underlying the Therapeutic Effects of Vitamin C against Cancer at Pharmacological Concentrations

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In pharmacological concentrations, ascorbic acid (vitamin C) acts like an optimized anti-cancer drug which kills cancer cells whilst leaving normal cells unaffected. Different mechanisms have been proposed to explain this behavior, however the underlying mechanism has remained elusive. We use a mathematical model, and the fact that ascorbic acid at pharmacological concentrations produces high levels of H_2O_2, to show that the produced H_2O_2 can in fact kill cancer cells and leave the normal cells unharmed. Based on our model we propose new strategies to enhance the therapeutic effect of ascorbic acid.

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Modeling and Pharmacokinetic Aspects for the Interaction between Beta Amyloid peptide and Choline Acetyltransferase and Acetylcholine Neurocycle and their relation to Alzheimer's and Parkinson's Diseases

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The interaction between Beta Amyloid peptides (βA) and the enzyme of choline acetyltransferase (ChAT) which is responsible for synthesizing Acetylcholine (ACh) neurotransmitter is investigated through two-enzyme/two-compartment model built previously. The presynaptic neuron is considered as compartment 1 while both synaptic cleft and the postsynaptic neuron are considered as compartment 2. The main objective of this work is to analyze the effect of βA inhibitor on ChAT enzyme in different situations. Therefore, different kinetic mechanisms are proposed to study the impact of the βA as an inhibitor on different species of the ChAT to study the nature of the inhibitory effect of the enzyme. It is found that the rate of ACh synthesis in compartment 1 has been reduced with the increase of feed concentration of βA with each pharmacokinetic mechanism in conjunction with the ACh in concentration in compartment 1.

The most severe effect occurs when βA acts as a noncompetitive inhibitor and can bind to all of the ChAT species in the reaction with the same affinity at high concentration of the inlet βA. Therefore, the oscillatory behavior dominates the ACh neurocycle and lead to disturbances for all state variables such as ACh, choline, acetate, and pH in each compartment. The irregular changes in all state variables of the system appeared through the mentioned oscillatory behavior could give a reasonable explanation for the effect of βA and the reduction of ACh levels in Alzheimer's and Parkinson's diseases.

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Weakly compressible tube flow with radially dependent viscosity and Navier slip at the wall

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Particle-based methods for blood flow applications have gained popularity in recent years, as they allow for the possibility of a more detailed description of the flow field, as well as a more fundamental understanding of the connection between particle-based interactions and the observed macroscopic flow properties. For a particle-based system whose dynamics obey the multiparticle collision (MPC) rule, the averaged macroscopic flow has been theoretically shown to be that of an ideal gas satisfying the Navier-Stokes equations of motion [1]. In other words, provided the compressibility is low, the average velocities of the particle-based system agree with the solution of the Navier-Stokes equations in the same flow geometry. Although particle-based flow through a rigid cylindrical tube is likely to exhibit small compressiblity effects, compressibility effects are built-in and the extent of the compressibility in a particular flow domain has to be understood and quantified if it is to be used for blood flow applications. In addition, although no-slip boundary conditions are commonly used for blood, blood was first proposed to satisfy slip at the wall in [2], and slip can easily be incorporated in particle-based methods [3]. Other applications of this work include flow through microfluidic devices, polymer melts, and extrudate-swell flows.

As a first step towards furthering our understanding of the role of slip and compressibility in the tube flow of blood, a first-order perturbation solution is obtained for steady, compressible flow with Navier-slip boundary conditions. Following [4], the viscosity is assumed to have the radially-dependent form

$$\mu = \mu_0 \left[1 + k - k\left(\frac{r}{R}\right)^n\right] \tag{1}$$

where μ_0 is the plasma viscosity, $k = 2.5h_m$, h_m is the maximum hematocrit at the tube center, R is the radius, and $n = 1$ and 2. The perturbation is performed on the non-dimensionalized, compressible, Navier-Stokes equations of motion whose viscosity satisfies (1). Following [5], a linear equation of state is assumed with compressibility number $\varepsilon = \frac{8\mu_0\beta UL}{R^2}$ used as the perturbation parameter. Here U is the velocity and β the isothermal compressibility.

In all cases considered, the leading order corresponds to incompressible, slip flow with only radial dependence in the axial velocity. The first-order correction depends on the aspect ratio $\alpha = R/L$ and Reynolds number $Re = \rho UR/\mu$, and also depends on the axial location. The extent of compressibility, slip, k and n-dependence on flow through a cylindrical tube are assessed, and results are compared to some existing experimental blood flow data.

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A Machine Learning Tool for Automated Image Segmentation

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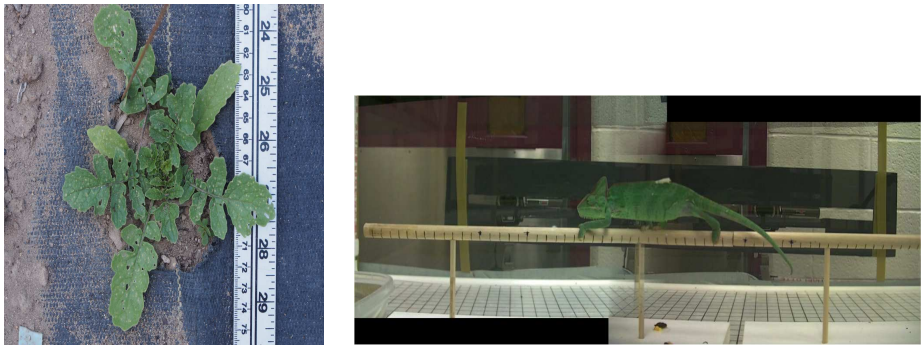
Image segmentation is the process of dividing pixels in an image into categories based on shared visual characteristics (e.g., color, texture, geometry, etc.). This is often an important first step in various applications in that the process partitions an image into subimages that are easier to analyze. Image segmentation is a challenging problem due to sensor-based noise, artifacts caused by motion, and partially observable objects due to obstruction. Numerous algorithms (e.g., level set, region growing, and graph-based methods) have been invented for image segmentation; however, there is no universal algorithm for segmentation of all images. In addition, image segmentation is not a fully-automated process.

We propose a machine learning tool for automated segmentation of a set of images. In particular, our technique starts by using an existing image segmentation algorithm to (semi-automatically) segment the first image in the data set. The next step is to use our multiobjective optimization technique for matching the segmented shapes in the initial image to the most similar shapes in the second image in the data set. Optimal shapes are determined based upon color, texture, geometry, and motion. This process is then repeated in order to segment the remaining images in the data set. Machine learning is used as the optimization process is ongoing in order to determine the most appropriate values for the weights of the relevant terms in the objective function for a set of images. We present results from testing our automated image segmentation tool on various sets of biological images [1, 2, 3].



(a) Plant Application [1] (b) Chameleon Application [2, 3]

Figure 1: Example image segmentation problems.

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[1] Image provided by A. Charbonneau as part of a study to quantify phenotypic differences between weedy and native radish populations, Michigan State University, Work in progress, (2013).

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Effect of fluid friction in fluid flow simulation in solid tumors

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It is known that more than 85% of human cancers involve solid tumors [1]. The numerical simulation of tumor growth has significant information for delivery of therapeutic agents to tumor sites. The fluid flow modeling of tumor includes different scales, from modeling blood flow through capillaries as microscale to modeling fluid flow in tissue as macroscale. In this work, the macroscale model of fluid flow in tissue is considered. In a macroscopic model, only the distribution of variables, such as interstitial pressure and concentration, over the length scale of the tumor radius is important, and microscopic characteristics, such as blood vessels, cells, and the interstitial matrix, are not involved directly in the model.

Darcy's law is one of the most famous models in fluid flow in porous media especially in tissues. Results obtained by Darcy's law show good agreement with experimental data [2, 3], but there are some limitations to the use of Darcy's law. It is shown that the friction within the fluid and exchange of momentum between the fluid and solid phases is neglected by Darcy's law. In this work, it is inspected how neglecting friction can effect on results by considering a more general model for porous media, Brinkman Equation.

A tumor tissue surrounded by normal tissue is simulated. For the sake of simplicity, solid tumors are considered here to be spherical. The radius of tumor is 20 % of total radius. Results obtained show that the interstitial pressure distribution is the same for both models. However, the velocity field is changed specially the profile of velocity in the tumor region because of considering friction within the fluid. Figure 1 shows velocity contours for two models.

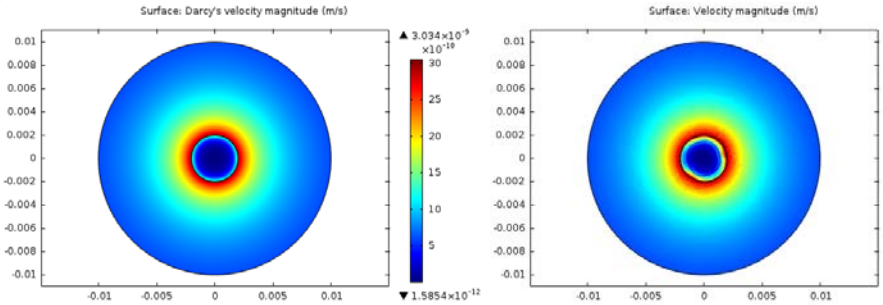

Figure 1: the velocity profile for two models. Darcy model (left) and Brinkman (right)

In spite of different results in velocity distribution, the investigation of results shows that there is no significant differences between two models. It is caused from macroscopic scale in which the capillaries are not considered; therefore, it is not necessary to consider a more complicated model for simulation tumor tissue when only the macroscopic scale is important.

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The Effects of Body Fluid on Cheyne-Stokes Respiration

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Cheyne-Stokes respiration (CSR) is a breathing pattern cycling between apnea (temporary breathing cessation) and hyperpnea (rapid and deep breathing). It is neurological in origin and is associated with the brain's monitoring of carbon dioxide levels in the blood. The fundamental features causing this periodic breathing are the sensitivity of the chemorecptors in the neck to CO_2 levels and the delay in the signal from the lungs to the receptors. CSR is analogous to trying to get warm water from the end of a long hose by adjusting a very responsive hot water faucet. The water is too cold so you open the hot faucet more, but after a short while the water is too hot so you close the faucet some, etc.

Clinical researchers hypothesize that fluid shifts in the body when changing from an upright to a recumbent position are a factor involved in the onset of CSR. A model of CSR that incorporates body fluid shifts fit to clinical measurements is presented and analyzed [1]. The model exhibits a super-critical Hopf bifurcation where the steady-state, representing normal breathing, becomes unstable and a stable periodic cycle, representing CSR, emerges. Two of the important parameters in the model are the gain, μ, (sensitivity) of the chemorecptors and the ventilation-perfusion ratio, r, (the ratio of the equilibrium ventilation rate to the blood flow rate). The latter of these is known to typically lie in a certain range for subjects at rest, however, the former parameter is purely a modelling construct and its value is not physically measurable. Hopf bifurcation curves are plotted in the (r,μ)-plane and their location is studied as a result of shifting the blood fluid parameters in the model, corresponding to being in the supine position. It is shown that these fluid shifts move the bifurcation curve significantly downward in the plane, which means that CSR will emerge at lower gain values. In addition, these shifts are more pronounced in male subjects than in female ones. These results are in agreement with clinical knowledge and support the hypothesis that body fluid shifts are a factor in the onset of CSR.

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The spatio-temporal spread of drug-resistant tuberculosis

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Tuberculosis is, after HIV/AIDS, the second largest cause of infectious disease induced death. It is estimated that in 2011, it killed 1.4 million people worldwide. Tuberculosis is also a disease of poverty, as contributing factors to its spread include poor and overcrowded living conditions, poor health conditions, etc. As a consequence, over 95% of new infections and deaths by tuberculosis occur in developping countries.

Tuberculosis is lethal in about one third of untreated cases, but treatment is now readily available. However, it is not always available to all in poorer countries where the incidence (number of new cases per unit time) is also high. Furthermore, treatment for active tuberculosis is lengthy, lasting from six months to a year. As a consequence, a number of patients withdraw from treatment. Not only is this detrimental to their health, it also promotes resistance (in the tuberculosis bacterium) to anti-tuberculosis agents. In recent years, strains of tuberculosis have been observed that are resistant not only to one, but also to two or more front line drugs. Multi-drug resistant tuberculosis (MDR-TB), which is resistant to at least two drugs, has been observed in virtually every country in the world. Extensively-drug resistant tuberculosis (XDR-TB), which is resistant to three or more front line drugs, is on the rise in several countries. Outbreaks of XDR-TB are particularly worrisome: as patients harbor a pathogen that is resistant to several of the most usual antituberculosis drugs, treatment is complicated and the mortality induced by the disease is therefore very high, reaching 100% in some epidemics.

On the other hand, immigration has become more and more frequent, with a clear gradient from poorer to richer countries. As an example, there are on average 250,000 new permanent residents and now almost 300,000 temporary workers in Canada each year. The four countries that contributed more than 10,000 new permanent residents per year on average in the last ten years are China, India, Pakistan and the Philippines. These countries also have high prevalences of tuberculosis infection, both drug-sensitive and resistant.

The usual paradigm is for rich countries to screen incoming new immigrants to detect active tuberculosis and to treat those who are latently infected upon arrival and develop active tuberculosis (the period of dormancy of the disease can be many years long, many individuals harboring the bacterium never become sick). However, this assumes implicitly that immigrants will remain in the country once they have arrived. This is not true in the modern world of cheaper and faster travel. Many immigrants return to spend extended periods of time in their home country or are visited by relatives (who are typically not screened). Residents of rich countries also travel more to poorer countries than they used to, whether for business or leisure.

To investigate these ideas, we formulate a model for tuberculosis in a single population that includes three strains: a drug-sensitive strain, MDR-TB and XDR-TB. We study the model mathematically and show, in particular, that the bifurcation structure of the whole model is governed by the behaviour of the XDR-TB strain. We then extend the model to a metapopulation setting, in which each country is a vertex in a multi-digraph, endowed with a system for the single population case. Weighted arcs between the vertices represent the rate of travel of individuals between the countries. We study the resulting large-scale system. Finally, we proceed to numerical experiments with realistic travel and population data.

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Mass Media effects on an Influenza Epidemic

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Influenza causes annual epidemics and occasional pandemics that have claimed millions of lives throughout history. Media reports affect social behaviour during epidemics and pandemics. Changes in social behaviour, in turn, affect key epidemic measurements such as peak magnitude, time to peak, and the beginning and end of an epidemic. The extent of this effect has not been realized. We employ agent-based Monte Carlo simulations to investigate the mean and variability in key epidemic measurements important to public health officials. A novel inclusion of mass media is developed through the addition of a mass media compartment in a Susceptible-Exposed-Infected-Recovered (SEIR) model. Multiple levels of social distancing are considered, media boredom and vaccination uptake. Sensitivity analysis is performed using Latin Hypercube Sampling and Partial Rank Correlation Coefficients. Systems of stochastic differential equations are also derived to compare to the stochastic agent-based Monte Carlo simulation. Data is used in place of the novel media equation in the model. The model results are compared with the data from the H1N1 pandemic in 2009.

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A mathematical model for the spread of ectoparasite-borne diseases

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A mathematical model is presented to simultaneously study the dynamics of ectoparasite infestation and infectious diseases spread by those ectoparasites. The system has four potential equilibria. We identify the reproduction numbers which determine whether the infectious or the non-infectious parasites can invade the population, and whether a population already infested by non-infectious parasites can be invaded by the infection. By using Lyapunov functions and persistence theory, we show that the solutions always converge to one of the equilibria, depending on the reproduction numbers. Hence the global dynamics is completely characterized by the reproduction numbers. We also give a description of the structure of the global attractor in all possible cases.

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Population-level effects of suppressing fever

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Fever is commonly attenuated with antipyretic medication as a means to treat unpleasant symptoms of infectious diseases. We highlight a potentially important negative effect of fever suppression that becomes evident at the population level: reducing fever may increase transmission of associated infections. A higher transmission rate implies that a larger proportion of the population will be infected, so widespread antipyretic drug use is likely to lead to more illness and death than would be expected in a population that was not exposed to antipyretic pharmacotherapies. We make these statements precise by analyzing mechanistic mathematical models and estimate the magnitude of the population-level effect for influenza; we find it is significant, causing an increase of 4% in the expected number of cases and deaths [95% CI: 0.12–10%].

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Optimal Infectious Disease Control

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The simplest model for the spread of an infectious disease in a population is a so-called susceptible-infected-removed (SIR) model (see [1, 2]). According to this model, a population (of a constant size N) is divided into three compartments: the susceptible S, the infected I and the removed (recovered and immune) R. It is usually assumed that all the newborn are susceptible (and hence are coming to compartment S), that the population size is approximately constant (that is, the demographic processes are considerably slower than the epidemic ones), and that a recovery implies the immunity of the individual. Interesting optimal control problems for SIR models were considered in [3, 4]. In this work, in order to control the spread of infection, we modified the system by adding to it three bounded controls, $p(t)$, $q(t)$ and $r(t)$. The model equations respectively are:

$$\begin{aligned} S'(t) &= \mu(1-p(t))N - \frac{\beta}{1+r(t)}S(t)I(t) - (\mu+q(t))S(t), \ t \in [0,T], \\ I'(t) &= \frac{\beta}{1+r(t)}S(t)I(t) - (\gamma+\mu)I(t), \\ R'(t) &= -\mu R(t) + q(t)S(t) + \gamma I(t) + \mu p(t)N. \end{aligned}$$

Here, $p(t)$ is vaccination of the newly born; $q(t)$ vaccination of the susceptible, and $r(t)$ is other "indirect" strategies aimed at a reduction of the incidence rate, such as quarantine or some precocious measures. The properties of our control models are investigated analytically. The optimal control problem of minimizing the number of the infected species at the terminal time T is stated and solved. The optimal solutions are obtained with the use of the Pontryagin Maximum Principle. Numerical results are presented to illustrate the optimal solutions.

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A Century of Transitions in New York City's Measles Dynamics

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Infectious diseases spreading in a human population can occasionally exhibit sudden transitions in their qualitative dynamics. Previous work has been very successful in predicting such transitions in New York City's measles incidence rates using the standard SIR model (*susceptible, infected, recovered*). This work relied on a data-set spanning 45 years [1], which we have extended to 93 years (1891-1984). We continue previous research in transition analysis on this larger data-set, and compare resonant and transient periods predicted to exist in NYC's measles incidence rates with those observed through a continuous wavelet transform of the data. We find good agreement between SIR predictions and observation, and in particular note the likely existence of previously unobserved hysteresis early in our new time-series.

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Modelling pre-emptive vaccination to prepare for bioterrorist attacks

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Though smallpox has been eradicated, the threat of its use for biological warfare or bioterrorism remains. Substantial vaccine-induced morbidity and mortality make pre-emptive vaccination controversial, and induce a conflict between self- and group-interests if vaccination is voluntary. Previously, this conflict has been explored numerically for a particular post-attack vaccination scheme. Here, we generalize previous work by considering several plausible post-attack vaccination scenarios and derive analytical formulae for the self- and group- optimal pre-attack vaccine coverages. We compare the expected increase in morbidity and mortality that results from voluntary vs imposed vaccination for each of the vaccination scenarios considered.

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Seasonal Modeling of Chronic Wasting Disease

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Force of infection, in most of disease models, remains unchanged while parameters may vary seasonally. We developed and analyzed a summer and winter susceptible-infected (SI) model with a seasonal change in the modal form of the force of infection. We applied it to chronic wasting disease (CWD) in deer. The model postulates an impulsive birth with density-dependent birth rate. We found the basic reproduction number as a weighted average of two reproduction numbers corresponding to the modes of transmission. We used parameter values for the model from data derived from the literature of CWD and deer ecology. Then, we conducted global and local sensitivity analyses of the basic reproduction number. Using the model, we explored the effectiveness of different culling strategies for the management of CWD. The main conclusion is that seasonal changes in behavior can lead to a vital change in the disease transmission mechanism and so to disease management.

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A multi-strain analysis of Neisseria meningitidis on the impact of immunization in Canada

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Neisseria meningitidis is a multi-strain pathogen that has 6 main serogroups which is highly prevalent in infants and teenagers. In Canada, serogroups B, C and Y are prevalent in the population with W-135 and A occurring from time to time and X very rarely[1]. Vaccines are used to prevent cases of invasive meningococcal disease (IMD; a condition occasionally caused by *Neisseria meningitidis*), which is has a high morbidity rate, even though *N. meningitidis* is typically carried asymptomatically. *Neisseria lactamica* is another pathogen in the same family as meningitidis but it is not associated with invasive meningococcal disease. However, *N. lactamica* has been shown to confer immunity to individuals against *N. meningitidis*[2]. There have been no multi-strain models that look at the dynamics of the six serogroups of *Neisseria meningitidis* and how the different serogroups have been impacted by immunization. We use an agent-based model to simulate the multi-strain pathogen transmission and assess the use of vaccine in a Canadian setting. Various vaccine schedules are assumed to show how age of vaccination impacts the prevalence of carriage as well as incidence of IMD[3]. Different types of vaccines such as a monovalent C vaccine, and quadrivalent ACWY are used and analysed to find an optimal vaccine program. In Canada, the quadrivalent ACWY vaccine is used to target serogroups A, C, W-135, and Y. According to model projections, the use of the ACWY vaccine will cause an increase in serogroup B infection due to strain replacement. If a monovalent vaccine is used, more than one strain will compete to replace the empty ecological niche, and replace the serogroup targeted by the vaccine.

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Pair approximation models of foot and mouth disease: Optimal culling and vaccination strategies, impact of vaccine waning; loss of natural immunity; disease re-introduction.

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Moment closure approximations, in particular, SEI (susceptible-exposed-infectious) pair approximations models have been designed, studied and used viz a viz empirical data to describe the spatial farm-to-farm transmission of foot and mouth disease (FMD). Such models have been utilized, not only as predictive tools, but also as means of modeling impacts of control measures against the spread of FMD: culling and vaccination- during outbreaks. However, farms that recover from FMD become susceptible again in the long run. Vaccines against foot and mouth disease do not confer life-long immunity, so a new outbreak in the same population of farms may lead to infection of previously vaccinated farms. Therefore we extend these models to SEIRV (susceptible-exposed-infectious-recovered-vaccinated) pair approximation models of FMD, thus incorporating impacts of loss of natural immunity and vaccine waning, in cases where disease importation is possible. In addition to during-outbreak-vaccination strategies used in previous studies, we consider impacts of prophylactic vaccination and measure optimal vaccination coverages that will prevent future outbreaks of foot and mouth disease. We present a spatially-oriented expression of the basic reproduction number, R_0 (a threshold value under which the disease is expected to die out), of foot and mouth disease as a function of rates of culling and vaccination, and seek optimal culling and vaccination strategies that minimize R_0. Upon re-introduction of FMD virus into a population of farms, the susceptible denominator now also constitutes previously vaccinated and recovered farms. Vaccine waning and loss of natural immunity lead to infection and reinfection of previously vaccinated and infected farms, respectively. Administration of optimal prophylactic vaccination is expected to eradicate the disease by preventing future outbreaks. We determine optimal IP (infected premises) culling and CP (contagious premises) culling rates that minimize cumulative number of infections, infection peak and the basic reproduction number. We also determined optimal prophylactic and ring vaccination (during outbreak) rates. The novelties of pair approximation models, compared to mean-field approximations are (i) their ability to capture the role of local correlations in a network of farms, and (ii) that they are mathematically tractable (this enables calculation of the basic reproduction number and hence determine conditions under which the disease can be contained). Small values of IP culling (relative to other model parameters), slightly reduce infection peak but delay disease eradication leading to increased cumulative number of infectious farms. On the other hand, vaccine CP culling significantly reduce infection peak and cumulative number of infectious farms. The findings of our research guide foot and mouth disease control policy.

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Seasonal dynamics in an SIR epidemic system

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In epidemic model, the cause of seasonality may vary from human force phenomena, like the succession of school terms and holidays. We consider a seasonally forced SIR epidemic model where periodicity occurs in the contact rate. The dynamics are described by a switched system. First, we prove the existence of an invariant domain D containing all periodic orbits. Then, using different scales in time and variables, we write the SIR model as a slow-fast system and establish the existence of a macroscopic attractor domain K, included in D. The existence of a unique harmonic solution is proved for any value of the magnitude of the seasonal forcing term which can be seen as an annual infection. Subharmonic solutions can be seen as epidemic outbreaks. Our theoretical results allow us to exhibit quantitative characteristics for epidemics.
We consider an SIR system, where the population is divided in susceptible $x(\tau)$, infective $y(\tau)$ and removed $r(\tau)$. Let $\beta(\tau)$ the rate of transmission, Infected individuals may recover at rate γ. Vital dynamics is taken into account by considering a natural mortality rate μ equal to birth rate; so the size of the population is constant abd $r(\tau)$ becomes irrelevant for the study. The dynamics write

$$\begin{cases} \frac{dx}{d\tau} = \mu(1-x) - \beta(\tau)xy \\ \frac{dy}{d\tau} = \beta(\tau)xy - (\gamma+\mu)y, \end{cases} \tag{1}$$

The transition from one season to the other is quasi-instantaneous since it is governed by periods of school terms and holidays, so we can do the approximation: the dynamics are governed by switching between two systems, where $\beta(\tau)$ is a T_τ-periodic switch signal defined as follows. Let

$$\delta_+ = 1+\delta, \quad \delta_- = 1-\delta, \quad \beta_+ = \beta_0\delta_+, \quad \beta_- = \beta_0\delta_-,$$

and $\beta(\tau)$ defined in $[0,T_\tau)$ by

$$\beta(\tau) = \begin{cases} \beta_+ & \text{for} \quad \tau \in [0, \theta T_\tau) \\ \beta_- & \text{for} \quad \tau \in [\theta T_\tau, T_\tau) \end{cases},$$

where β_0 is the mean contact rate, $\delta \in (0,1)$ the seasonal forcing, $\theta \in (0,1)$ and θT_τ the high epidemic period. According to data in the literature, one can consider the parameters be ranked based on their order of magnitude:

$$0 < \mu << \delta < 1, \quad 0 < \theta < 1, \quad 0 < \gamma < \beta_0.$$

We consider μ as a small parameter and do the change of state variable $y = \mu Y$, system (1) becomes

$$\begin{cases} \frac{dx}{d\tau} = \mu(1 - x - \beta_\pm xY) \\ \frac{dY}{d\tau} = (\beta_\pm x - \gamma - \mu)Y. \end{cases} \tag{2}$$

Since μ is a small parameter, system (2) is slow-fast system and we shall study the dynamic of system (2) in the framework of singular perturbation theory. Here the fundamental tools are Thikonov's theorem for convergence of solutions of slow-fast system and averaging to study periodic motions.

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Target Reproduction Number and Its Applications to Infectious Disease Control

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A new quantity called the target reproduction number is defined in [1] to measure control strategies for infectious diseases with multiple host types such as waterborne, vector-borne and zoonotic diseases. The target reproduction number includes as a special case and extends the type reproduction number [2, 3] to allow disease control strategies that target contacts between host types. Relationships among the basic, type and target reproduction numbers are established. Examples of infectious disease models from the literature are given to illustrate the applications of the target reproduction number.

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The Spread of Infectious Disease with Imported Infections

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Most models for the spread of an infectious disease have a disease-free equilibrium. This fails to be the case if infected individuals enter from the outside. This can happen if there is immigration of infectives into the region being studied.

Here, we consider models where infected individuals enter the population. An immediate consequence is that there is no disease-free equilibrium. Additionally, there is no basic reproduction number as that quantity is defined by the behaviour near a disease-free equilibrium.

For the models considered, we determine the global stability of the endemic equilibrium through the use of a Lyapunov function.

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The impact of the Anopheles mosquito lifestyle, feeding and reproductive habits in the transmission dynamics of Malaria-implications for control

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Malaria deaths continue to drop, but, remain a burden in many countries, killing mostly children. Mathematical models have extended our understanding of the biology and transmission dynamics of malaria, dating back to the Ross-Macdonald model. However, most models either treat the mosquito population density as a constant or do not model the reproductive gains that accrue to the mosquito's population as a result of its lifestyle, feeding and reproductive habits, as well as its interaction with the human population. The interaction between mosquitoes and humans introduce high variability in the mosquito population density and this variability affects both the mosquito population and the malaria disease dynamics (see Refs. [1, 2, 3]). This talk will highlight how the lifestyle of the *Anopheles* mosquito and the interaction between the mosquito and humans affect malaria transmission dynamics and introduce complexities not previously observed in deterministic continuous time models. Implications for malaria control will also be discussed.

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Sustained and transient oscillations induced by delayed antiviral immune response in an immunosuppressive infection model

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Sustained and transient oscillations are frequently observed in clinical data for immune responses in viral infections such as human immunodeficiency virus, hepatitis B virus, and hepatitis C virus. To account for these oscillations, we incorporate the time lag needed for the expansion of immune cells into an immunosuppressive infection model. It is shown that the delayed antiviral immune response can induce sustained periodic oscillations, transient oscillations and even sustained aperiodic oscillations (chaos). Both local and global Hopf bifurcation theorems are applied to show the existence of periodic solutions, which are illustrated by bifurcation diagrams and numerical simulations. Two types of bistability are shown to be possible: (i) a stable equilibrium can coexist with another stable equilibrium, and (ii) a stable equilibrium can coexist with a stable periodic solution.

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The Effects of Mass Gatherings on the Spatial Spread of an Epidemic

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In this talk, we will investigate the spatial spread of an infectious disease in conjunction with a mass gathering. Mass gatherings take place when a large number of people from different locations visit a particular region during a particular time period. Such activity plays a crucial role in the epidemic spread as travel speeds up the spatial spread of an epidemic and crowded conditions accelerate the transmission and infection of the disease. We construct a mathematical model to study the epidemic spread with a periodic mass gathering involved. Our investigation reveals the effects of mass gathering on an epidemic spread.

Theory and Applications in Finance (SS-MFMCR)

Organizers:
Joe Campolieti (Wilfrid Laurier University)
Adam Metzler (Wilfrid Laurier University)

This minisymposium covers a diverse range of topics in contemporary financial mathematics. This could include, but is not necessarily limited to, credit risk, pricing and hedging exotic derivatives, correlation modeling, numerical methods for PDE/PIDE problems in finance, simulation methods in finance, energy derivatives, market microstructure and problems in financial regulation.

Numerical Methods for Computationally Intensive Problems in Mathematical Finance (SS-CF)

Organizers:
Duy-Minh Dang (UW)
Ken Jackson (University of Toronto)

The rapid growth and diversity of the financial markets over the past few decades has spawned many intellectually challenging and computationally intensive problems to be solved. These challenging problems are now spawning radical changes in computational methods in finance: more mathematically sophisticated and efficient computational methods are in great demand for the valuation and risk-management of complex financial instruments. This special session will bring together researchers who will discuss recent developments in efficient computational algorithms for the numerical solution of computationally intensive problems in mathematical finance. These problems range from pricing of multi-asset options under a regime switching or uncertain volatility model, or cross-currency foreign exchange interest rate derivatives, to computing the loss distribution of credit portfolios. The computational techniques used include asymptotic expansion-based approximation methods, partial differential equations and Monte-Carlo simulations, as well as utilization of emerging computer architectures, such as Graphics Processing Units (GPUs), to further increase the efficiency of the numerical methods.

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Hedging Costs for Variable Annuities

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A general methodology is described in which policyholder behaviour is decoupled from the pricing of a variable annuity based on the cost of hedging it, yielding two sequences of weakly coupled systems of partial differential equations (PDEs): the pricing and utility systems. The utility systems are used to generate policyholder withdrawal behaviour, which is in turn fed into the pricing systems as a means to determine the cost of hedging the contract. This approach allows us to incorporate the effects of utility-based pricing and factors such as taxation. As a case study, we consider the Guaranteed Lifelong Withdrawal and Death Benefits (GLWDB) contract. The pricing and utility systems for the GLWDB are derived under the assumption that the underlying asset follows a Markov regime-switching process. An implicit PDE method is used to solve both systems in tandem. We show that for a large class of utility functions, the two systems preserve homogeneity, allowing us to decrease the dimensionality of solutions. We show that the associated control for the GLWDB is bang-bang, under which the work required to compute the optimal strategy is significantly reduced. We extend this result to provide the reader with sufficient conditions for a bang-bang control for a general variable annuity with a countable number of events (e.g. discontinuous withdrawals). Homogeneity and bang-bangness yield significant reductions in complexity and allow us to rapidly generate numerical solutions. Results are presented which demonstrate the sensitivity of the hedging expense to various parameters. The costly nature of the death benefit is documented. It is also shown that for a typical contract, the fee required to fund the cost of hedging calculated under the assumption that the policyholder withdraws at the contract rate is an appropriate approximation to the fee calculated assuming optimal consumption.

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Interconnected Balance Sheets, Market Liquidity, and the Ampification Effect in a Financial System

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This paper investigates the amplification effect of a financial system to develop individual defaults to a systemic catastrophe. In our model, the financial institutions interconnect via two mutually stimulating channels: their balance sheets are linked directly by holding debt claims against each other; they share the market liquidity to liquidate assets to meet debt liabilities when they face distress. We develop a network-based approach to characterize how the topological structures of the system and asset liquidation interact with each other to amplify the systemic risk. We propose two multipliers, network multiplier and liquidity multiplier, to capture the above amplification effects. We find that the amplification magnitude is largely determined by the eigenvalues of the liability matrix of the financial system, which provides a strong theoretical justification to some eigenvalue-based systemic risk measures in the existing literature. The model has a significant computational advantage and can be solved efficiently through the linear-complementarity-technique based fixed-point algorithm. This research also builds up a close connection between the study of financial systemic risk and the literature of stochastic network. Furthermore, we examine the effects of varying other important modeling parameters, including external economic environment, leverage level of the financial institutions, and liquidity nature of the assets.

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Hedging Bond Returns with Equity

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Typically, the most efficient and common way to hedge credit risk is through a credit derivative. However for many credit markets, such as High Yield or Emerging Market debt, credit derivatives may be too illiquid to be an effective hedge, or they might not be traded at all. In this talk, I will discuss some strategies for hedging the credit risk of a bond through the equity markets. This leads to the concept of a bond-to-equity hedge ratio. While the hedge ratio itself is model independent, its computation is dependent on a credit risk model. I discuss and compare the behavior of the hedge ratio for a variety of models, including Merton and Black-Cox, but also more complicated ones such as Moody's PD-LGD correlation model.

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Long-dated foreign exchange interest rate derivatives: modeling, computational challenges, and parallel computation via a PDE approach

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In the current era of wildly fluctuating exchange rates, cross-currency interest rate derivatives, especially long-dated foreign exchange (FX) interest rate (IR) hybrid derivatives, are of enormous practical importance. In this talk, we discuss modeling issues, highlight computational challenges, and present a parallel algorithm based on a Partial Differential Equation (PDE) approach for pricing long-dated FX-IR hybrid derivatives.

As an illustrative example, we focus on Power-Reverse Dual-Currency (PRDC) swaps, one of the most widely traded and liquid FX-IR hybrid derivatives, with a popular exotic feature, namely FX Target Redemption (FX-TARN). These products are exposed to moves in both the spot FX rate and the interest rates of the domestic and foreign currencies. We discuss the modeling of PRDCs using two one-factor Gaussian models for the two stochastic interest short rates, and a one-factor FX model for the spot FX rate. This results in a three-dimensional time-dependent parabolic PDE for the price of the PRDC swap. Challenges in pricing PRDCs with FX-TARN feature via a PDE approach arise from (i) the high-dimensionality of the model PDE, and (ii) the path-dependency of the FX-TARN provision.

Our PDE pricing framework for FX-TARN PRDC swaps is based on partitioning the pricing problem into several independent pricing sub-problems over each time period of the swap's tenor structure, with possible communication at the end of each time period. Finite difference methods on non-uniform grids are used for the spatial discretization of the PDE, and the Alternating Direction Implicit (ADI) technique is employed for the time discretization. Our implementation of the PDE pricing procedure on a cluster of Graphics Processing Units (GPUs) involves (i) assigning, with the help of MPI, each independent sub-problem to a different GPU, (ii) efficiently solving each independent sub-problem on its GPU via a parallelization of the ADI timestepping technique, and (iii) utilizing MPI for the communication between pricing processes at the end of each time period of the swap's tenor structure. Numerical results showing the accuracy and efficiency of the parallel PDE pricing methods, as well as possible extensions of this work, are provided.

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Multiple barriers and assets in Financial Mathematics

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In this talk we review recent mathematical results for multidimensional stochastic processes in the presence of multiple barriers. We study the distribution/density function of the minimums $(\min_{0<s<t} Y_1(t),\ldots,\min_{0<s<t} Y_n(t))$ and endpoints $(Y_1(t),\ldots,Y_n(t))$ of a n-dimensional Brownian vector (see [6]).

$$\begin{aligned} P \quad (\quad & Y_1(t)\in dy_1,\ldots,Y_n(t)\in dy_n, \min_{0<s<t} Y_1(s)>m_1,\ldots,\min_{0<s<t} Y_n(s)>m_n) \\ = \quad & p\,(y_1,\ldots,y_n,m_1,\ldots,m_n,t)\,dy_1\ldots dy_n, \end{aligned} \tag{1}$$

We pay special attention to the case $n=3$ (see [1]), here the targeted function p satisfies a PDE with the following initial and boundary conditions:

$$\frac{\partial p}{\partial t}(y,t) = -\sum_{i=1}^{3}\alpha_i\frac{\partial p}{\partial y_i}(y,t)+\frac{1}{2}\sum_{i=1}^{3}\sigma_i^2\frac{\partial^2 p}{\partial y_i^2}(y,t)+\sum_{i<j}\sigma_i\sigma_j\rho_{ij}\frac{\partial^2 p}{\partial y_i\partial y_j}(y,t). \tag{2}$$

$$p(y_1,y_2,y_3,t=0)=\delta(y_1)\delta(y_2)\delta(y_3), \tag{3}$$

$$\begin{aligned} p(y_1=m_1,y_2,y_3,t) &= 0,\\ p(y_1,y_2=m_2,y_3,t) &= 0,\\ p(y_1,y_2,y_3=m_3,t) &= 0. \end{aligned} \tag{4}$$

The Method of Images and ansatz solutions are used to find closed-form expressions to this problem. A generalization accounting for stochastic volatility is also presented in dimensions two and three (see [4], [3] and [5]). The usefulness of these results in finance is explored (see [2]) while new financial products are defined and closed-form analytical solutions are presented (see [5]).

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Trends and trades

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In this work, we build trend following algorithms based on the sequential statistical rules such as the Cumulative sum (CUSUM) and the Sequential probability ratio test (SPRT). We draw the connections between these statistics and the problem of online statistical surveillance and quality control which dates back to the 1930s. We focus on the cumulative sum statistic that has traditional been used for the online detection of abrupt changes in the distribution of sequences of observations. We study its construction and examine its properties. We also draw its connections to the well-known path dependent statistics used to capture sudden market drops/crashes and upward trends, namely the maximum drawdown and the maximum draw-ups. We proceed to construct trend following algorithms based on the CUSUM statistics and use them to trade on the 5-year US note sold at auction. We analyze the performance of such a rule which is seen to be most profitable during times of market instability and present the results of its performance in detail. We finally discuss other statistics of interest, such as the speed of reaction of the CUSUM statistic, and the way in which they can help us improve the performance of our proposed algorithm.

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Illiquidity and Insolvency: a Double Cascade Model of Financial Crises

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In the view of many experts, the proper definition of systemic risk is now seen to comprise two distinct facets. The traditional view that systemic risk is primarily the risk of cascading bank defaults has evolved into the view that systemic risk involves both cascading bank defaults as well as liquidity shocks, and that both types of shocks impair the functioning of the remaining undefaulted banks. In current models of systemic risk, for example [1], [2] and [3], these two facets, namely illiquidity and insolvency, are often treated as two distinct and separate phenomena.

This talk will describe a "deliberately simplified model" of insolvency and illiquidity in financial networks that integrates these two facets as two faces of the same coin. On the default side of the coin, insolvency of a given bank will create a shock to the asset side of the balance sheet of each of its creditor banks. Under some circumstances, such "downstream" shocks can cause further insolvencies that may build up to create a global insolvency cascade. On the flip side, in a stress cascade, illiquidity that hits a given bank will create a shock to the liability side of the balance sheet of each of its debtor banks. Under some circumstances, such "upstream" shocks can cause further illiquidity stresses that may build up to create a global illiquidity cascade. The pivotal question one wishes to address is: in a given financial network, what effect does the illiquidity or insolvency of a single firm have on the liquidity or solvency of other banks in the system?

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A convolution method for numerical solution of backward stochastic differential equations

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We propose a new method for the numerical solution of backward stochastic differential equations (BSDEs) which finds its roots in Fourier analysis. The method consists of an Euler time discretization of the BSDE with certain conditional expectations expressed in terms of Fourier transforms and computed using the fast Fourier transform (FFT). The problem of error control is addressed, we consider the extension of the method to reflected BSDEs, and some numerical examples are considered from finance demonstrating the performance of the method.

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Computation of the Loss Distribution Based on the Structural Model for Credit Portfolios

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Credit risk analysis and management at the portfolio level is a challenging issue for financial institutions due to their portfolios' large size, heterogeneity and complex correlation structure. In this paper, we propose several new asymptotic methods and exact methods to compute the distribution of a loan portfolio's loss in the CreditMatrics framework. For asymptotic methods, we give an approximation based on the Central Limit Theorem (CLT), which gives more accurate approximations to the conditional portfolio loss probabilities compared with existing approximations. To further increase the accuracy of approximations for lumpy portfolios, we introduce a hybrid method which combines an asymptotic approximation with Monte Carlo simulation. For exact methods, we improve the efficiency by exploiting the sparsity that often arises in the obligors' conditional losses. A sparse convolution method and a sparse FFT method are proposed, which enjoy significant speedups compared with the straightforward convolution method. We also construct truncated versions of the sparse convolution method and the sparse FFT method to further improve their efficiency. To balance the aliasing errors and roundoff errors incurred in the truncated sparse FFT method, an optimal exponential windowing approach is developed as well.

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Efficient Monte Carlo Simulation For Integral Functionals of Brownian Motion

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In the paper we propose a new method of generating Brownian motion sample paths with the objective of constructing efficient methods of simulation to evaluate expectations of the form

$$E[G(\int_0^T g_1(t,W(t))dt,\ldots,\int_0^T g_r(t,W(t))dt,W(\cdot))], \tag{1}$$

where $G, g_1, \ldots, g_r$ are given functions and $W(\cdot)$ represents a path of a standard Brownian motion $\{W(t); t \in [0,T]\}$. One of the main difficulties when dealing with integration problems of this form is their high dimensionality, stemming from the fact that to represent a Brownian motion path we need a large number of independent variables. Because of this, Monte Carlo simulation methods prove to be particulary useful, as their $O(N^{-1/2})$ convergence rate, where N is the number of samples, does not depend on the dimension of the problem. However this rate can be too slow for many applications, and hence numerous techniques have been considered to reduce the simulation error.

In order to increase efficiency of integration methods, we propose a novel method of reducing the dimension of the problem, and then we replace the random numbers that drive the simulation by a sequence of deterministic points, called low-discrepancy points, that cover the space more uniformly. It is known that such methods, referred to as quasi-Monte Carlo, have the potential to increase the convergence rate from $O(1/\sqrt{N})$ to $O(\log(N)^d)/N)$, where d is the dimension of the problem. This is a significant gain in efficiency, but only for problems of small to medium dimension. Reducing the dimension, by finding the right set of coordinates that would capture a large part of the overall variability of a given integrand, is a challenging problem. In the context of quasi-Monte Carlo methods, it is usually studied by using the concept of effective dimension, and practical results are typically obtained by applying a particular linear transformation to the vector of input variables.

We approach this problem by treating the important coordinates as variables for stratification. We show that for expectations of the form (1) we may significantly increase efficiency of the simulation method by combining the Brownian bridge construction with conditioning on integrals along paths of the process. In particular, our analysis suggests that instead of conditioning on $(W(t_1),W(t_2),\ldots,W(t_d))$ we should rather condition on the vector that includes only half of these values but supplemented with integrals. The main reason for the better performance of the latter method is the fact that conditioning on $(W(t_2),W(t_4),\ldots,W(t_d))$ reduces the integration problem to a series of similar problems but over shorter time intervals. Since smooth functions over shorter intervals can be more accurately approximated by linear functions, conditioning on integrals $\int_{t_i}^{t_{i+2}} W(s)ds$ becomes a very effective way of capturing variability. We formalize this intuition by proving that as we increase d then the amount of variability captured by $(W(t_2),W(t_4),\ldots,W(t_d),\int_0^{t_2} W(s)ds,\ldots,\int_{t_{d-2}}^{t_d} W(s)ds)$ is of order better than the one for the Brownian bridge construction.

An area of possible applications of the proposed method is modern finance, where expectations of the form (1) arise either directly or can be obtained through some transformations of a similar problem but defined in terms of a more general diffusion process. Such situations include, for example, the problem of pricing in the context of interest rate models and stochastic volatility models. Expectations of the form (1) also appear in the context of statistical inference for diffusion processes. In the paper we illustrate the method by applying it to the problem of pricing of Asian options, and our numerical results suggest that the method has considerable potential for a substantial reduction of the simulation error.

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An unconditionally monotone numerical scheme for the two factor uncertain volatility model

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In uncertain volatility model, the volatility of the risky asset is assumed to lie within a range of values. As such, prices obtained under a no-arbitrage analysis are no longer unique, and pricing in uncertain volatility models involves nonlinear partial differential equations, known as Hamilton-Jacobi-Bellman (HJB) partial differential equations (PDEs).

In this paper, we first develop a fully implicit, unconditionally monotone finite difference numerical scheme for two factor uncertain volatility models. Consequently, there are no time step restrictions due to stability considerations. The discretized algebraic equations are solved using a policy iteration. Our discretization method results in a local objective function which is a discontinuous function of the control. Hence some care must be taken when applying policy iteration. Furthermore, one difficulty is the monotonicity preserving approximation of the cross derivative in the PDE. We use a suitable wide stencil method to ensure monotonicity for our problem. Our numerical scheme is l_∞-stable, consistent in the viscosity sense, and monotone. Thus, our numerical scheme guarantees convergence to the viscosity solution.

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Hitting Times of Integrated Diffusions

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We construct a link between the first hitting time of the integral functional of a time-homogeneous diffusion to a fixed level, and the time integral of a related diffusion. This allows us to establish probabilistic results concerning these hitting times. We also discuss the simulation of such problems. This is joint work with Zhenyu Cui and extends work of Metzler (2012) on the Laplace Transform of the hitting times of integrated geometric Brownian Motion.

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Explosive behavior in a log-normal interest rate model

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The talk considers an interest rate model with log-normally distributed rates in the terminal measure in discrete time. Such models are used in financial practice as parametric versions of the Markov functional model [1, 2], or as approximations to the log-normal Libor market model [3]. This model is also similar to the Black, Derman, Toy model [4], up to the difference that the log-normal distributional assumption for the short rate is formulated in the terminal measure, as opposed to the risk-neutral (spot) measure. In a previous paper [5] it was shown that the model can be solved exactly, and that the exact solution displays two distinct regimes, at low and high volatility, with different qualitative behaviour. The two regimes are separated by a sharp transition, which is similar to a phase transition in condensed matter physics. The same phenomenon was observed [6] in a similar model with mean-reversion, which is the terminal measure analog of the Black, Karasinski model.

The talk considers the implications of the phase transition for the pricing of interest rates derivatives in this model. The shape of the Libor probability distribution function (in a measure where it is simply related to caplet prices) has a qualitative change at the critical volatility. For sufficiently small volatility this distribution has a usual humped shape, but it collapses to very small Libor values at the critical volatility, in addition to developing a long tail. This effect is visible in the caplet smile, which is log-normal to a good approximation for small volatility, but develops a non-trivial caplet skew in the large volatility phase. In addition, the moments of the Libor distribution function have sharp turning points in volatility. These effects limit the applicability of the model for describing an interest rate model with log-normal caplet smile, and define an upper limit on the volatilities for which the model behaves as intended.

In the large volatility phase, certain expectation values and convexity adjustments have an explosive behavior, which occurs at a sharply defined value of the volatility. These effects are due to contributions to the expectation values from a region in the state variable which is usually assumed to be unimportant in practice, as it associated with very large interest rates $\gg 100\%$. This region is usually truncated off in tree and finite difference implementations of the model, or is very poorly sampled in Monte Carlo simulations, unless impractically large numbers of paths are used. This implies that usual numerical implementations of the model do not capture correctly its behavior in the large volatility phase. The talk is based on the paper [7].

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A Bias-Reduction Technique for Monte Carlo Pricing of Multiple-Exercise Options

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We present a method for reducing the bias inherent in Monte Carlo estimators of multiple-exercise contingent claim prices. To demonstrate our approach, we employ the Forest of Stochastic Trees, a recently proposed tool for valuing multiple exercise options [1,2]. Its option value estimators are biased, analogous to the original Stochastic Tree estimators generated for valuing American style options. The bias-reduction technique presented is an extension of recent work [3,4] for American option value estimators to similar estimators for multiple exercise options. Using large-sample theory, we derive an approximation to the bias at each exercise opportunity which is then subtracted from the uncorrected estimators resulting in bias-corrected estimators. This approach to bias correction is independent of dimensionality and holds for general asset-price processes and payoffs.

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Delayed Heston Model: Improvement of Vol Surface and Hedging of Vol Swaps

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We present a new variance drift adjusted version [2, 4] of the Heston model [1] which leads to significant improvement of the market volatility surface fitting (compared to Heston). The numerical example we performed with recent market data shows a significant (44%) reduction of the average absolute calibration error (i.e., average of the absolute differences between market and model implied Black-Scholes volatilities) (calibration on Sep. 30th 2011 for underlying EURUSD). The main idea behind our model is to take into account some past-dependent history (a.k.a. delay) of the variance process in its (risk-neutral) diffusion. We also focus on volatility swap pricing and hedging [3, 4].

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Mathematics of Human Placenta: A Window into Fetal Origins of Adult Disease (SS-MHP)

Organizers:
Carolyn Salafia (Placental Analytics)
Oleksandr Shlakhter (Alberta Health Services)
Michael Yampolsky (University of Toronto)

Understanding how developmental problems of the fetus affect adult health risks is an important public health goal. Human placenta faithfully reflects abnormalities of fetal growth. Modeling placental growth and quantifying its vascular structure is a rich subject offering many exciting mathematical problems. The goal of the session is to bring together mathematicians and medical scientists working in this field.

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Metabolic Scaling Law for Mouse Fetal and Placental Weight

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In humans the fetal birth weight does not scale linearly with the weight of the placenta, but exhibits an allometric scaling consistent with the Kleiber's metabolic scaling law, so that placenta weight (P) is proportional to the fetal birth weight (F) raised to the scaling exponent of 0.75 ($P \sim F^{0.75}$) (Refs. [1, 2]). The mouse is a common animal model for studying genetic and physiological backgrounds of placental development, function and pathologies. The most accessible values to evaluate function of mouse placenta in experimental conditions (at most gestational ages) are placental and fetal weights. However, to date it has not been known whether the normal relationship between placental and fetal weight in mouse is linear or not.

To answer this question, we analyzed 163 embryos and corresponding placentas from 12 embryonic day 12.5 litters of CD1 wild type mice. Here we show that the mouse mid-gestation placental weight has a power-law scaling relationship with the fetal weight, and the value of the scaling exponent is approximately 0.72, similarly to the scaling of placental and birth weights in humans. The scaling relationship in wild type mice allows us to quantify the deviation from normal placental structure and function in experimental models that study placental response to genetic changes and/or environmental cues. Moreover, combined with a thorough histological analysis it constitutes a useful tool providing a more complete picture of both functional and structural placental changes.

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Modeling Oxygen Transport in the Inter-Villous Space of the Human Placenta

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The human placenta governs the exchange of oxygen, carbon dioxide, nutrients and water between the mother and the fetus. Due to its complex geometrical structure, both mathematical modeling and numerical simulations are required to describe the exchange processes going in it.

The maternal part of the human placenta is a blood basin into which maternal blood is delivered by spiral arteries and which is drained by maternal veins. The fetal part has a much more complicated tree-like structure which is immersed into the maternal blood basin anchoring to its basement and supporting the placenta shape. While fetal blood flows through capillaries inside the fetal villi, maternal blood percolates through the same arboreous structure on the outside. It is at the surface of this tree structure in its smallest parts that the exchange with the passing by maternal flow takes place.

The present model of a placental exchange unit consists of a large cylinder representing the intervillous space filled with maternal blood. This cylinder contains multiple smaller parallel cylinders which represent fetal villi. Although such geometrical representation might appear simple, it captures some important aspects of the role of the geometry in the system and shows directions for future development of the topic.

The flow of maternal blood in the model is oriented along the main axis of the system. In the perpendicular plane oxygen is only redistributed by molecular diffusion. Uptake takes place at the boundaries of the small cylinders. Its rate is proportional to the membrane permeability and to the oxygen concentration in the maternal region. The flow is considered to be laminar with slip condition on all boundaries, so that the velocity profile in a cylinder cross-section plane is flat. No account for oxygen-hemoglobin reaction curve or fetal blood flows is given.

The main questions that we address in this study are: (i) Is there an “optimal” villous tree geometry (in a sense to be defined)? (ii) What are the important parameters which influence oxygen transfer efficiency?

Numerical and theoretical calculations of fetal oxygen uptake as a function of the density of the villi show the existence of a maximal uptake at a density of the villi of around 50 %. Comparison of the result with histomorphometric studies shows a good correlation with the experimental data relative to the biological variance and errors. The influence of the choice of physiological parameters such as blood flow velocity on the position of the maximum peak is also studied.

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Human Placenta - The Interface for Two Vascular Systems

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The human placenta goes through a complex developmental sequence from implantation to delivery. Many have suggested that the developmental patterns have similarities to the fetal organs under development. The role of oxygen, nutrients and cytokines/chemokines will be examined as well the vascular responses in the term human placenta under in vitro dual perfusions. Studies of both the early and term responses of the placenta will be discussed and possible roles for vascular pattern development and function using albunex, nanoparticles and IgGs.

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Translating Measures of Placental Shape into Predictors of Infant and Childhood Health

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Our multidisciplinary team draws on the disciplines of mathematics, physics, pathology, and epidemiology in studying the role of placental shape as a predictor of infant and child health outcomes. Our work has collectively demonstrated that more nuanced and quantified measures of the placenta, derived from principles of mathematical and physical modeling, can predict a range of infant and childhood outcomes. From my perspective as an epidemiologist, I will describe the methods of data collection and analysis used by our team to study the effects of placental shape on outcomes. I will "translate" the measures of shape 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.

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Why placental shape matters: a research trajectory

Salafia C., Yampolsky M., Misra D., Miller R., Schwartz N.

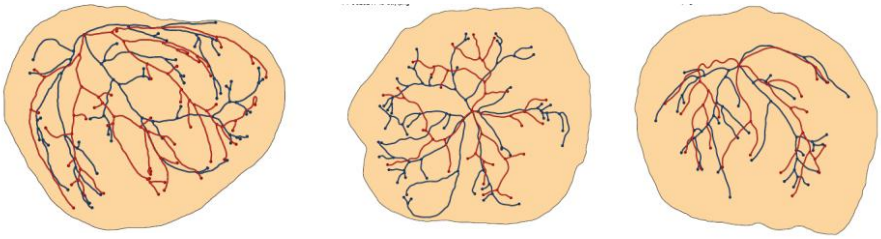
The last 7 years have seen an explosion in the ability to measure the placenta and from those measures, understand its growth in health and disease. A summary of highlights of analyses based on standard ruler-based placental measures, and image based novel approaches will be distributed at the session.

Chorionic vascular surface network analyses and their implications for placental function and fetal health will be discussed.

We have recently completed novel analyses of the chorionic surface vasculature in 33 Early Autism Risk Longitudinal Investigation (EARLI, high-autism risk) placentas compared 76 unselected National Children's Study (NCS) placentas. In summary, EARLI placentas as a group show significant placental chorionic surface vascular network differences, including reduced number of chorionic surface vascular branch generations, branch and terminal vascular points and reduced mean vessel caliber as compared to NCS placentas. In addition, in EARLI placentas as a group, chorionic surface arteries, but not chorionic surface veins, terminate further from the surface perimeter, and have greater variability in that distance, and the distances between chorionic surface arteries and chorionic surface veins throughout their course on the chorionic surface are both greater and have greater variability. Below left is an "average" NCS placental surface vascular network, center an EARLI placental surface vascular network 1SD above the mean surface vascular density, and right, an "average" EARLI placental surface vascular network. The implications for ASD and for other fetal, childhood and adult health risks will be discussed.

We have also demonstrated increased irregularity of placental chorionic surface shape, with umbilical cord insertion sites located closer to the placental chorionic surface perimeter (more eccentric umbilical cord insertions, Table 2). Our empirical models and direct research indicate that these features have their origin before the mid trimester.

Below left is an "average" NCS placental surface vascular network, center an EARLI placental surface vascular network 1SD above the mean surface vascular density, and right, an "average" EARLI placental surface vascular network.



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Is the placental disk really an ellipse?

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The mean surface shape of placenta is round and common abnormalities of shape are associated with vascular abnormalities and reduced placental functional efficiency. A long-standing approach is to describe shapes as elliptic, and to quantify them by “length” and “breadth”. We test this description in two cohorts: National Collaborative Perinatal Project and Pregnancy, Infection and Nutrition Study. We conclude that quantifying placental shape as elliptic is ambiguous and problematic. The “breadth” of the placenta should be interpreted as a combination of two different measurements: placental size and irregularity of the placental surface. It has no intrinsic functional significance.

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Optimal transport and the placenta

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The optimal transportation problem aims at finding an optimal way to transport a given probability measure into another. In contrast to the well-known Monge-Kantorovich problem, the ramified optimal transportation problem aims at modeling a branching transport network by an optimal transport path between two given probability measures. Transport networks with branching structures are observable not only in nature as in trees, blood vessels, river channel networks, lightning, etc. but also in efficiently designed transport systems such as used in railway configurations and postage delivery networks. An important feature of such a transport path is to favor transportation in groups via a nonlinear (typically concave) cost function on mass. An optimal transport path can be viewed as a geodesic in the space of probability measures with a suitable metric. It typically has a tree-shaped branching structure.

The goal of this talk is to introduce the use of ramified optimal transport modeling in studying the expected effects of (i) placental size, (ii) placental shape and (iii) the position of insertion of the umbilical cord on the work done by the foetus' heart in pumping blood across the placenta. We simulate a vascular tree structure, for each placenta, in a simplified form by an idealized optimal transport network. The computer algorithm finds a nearly optimal transport network for the data provided for each placenta. A typical one is similar to the left one of Figure 1.

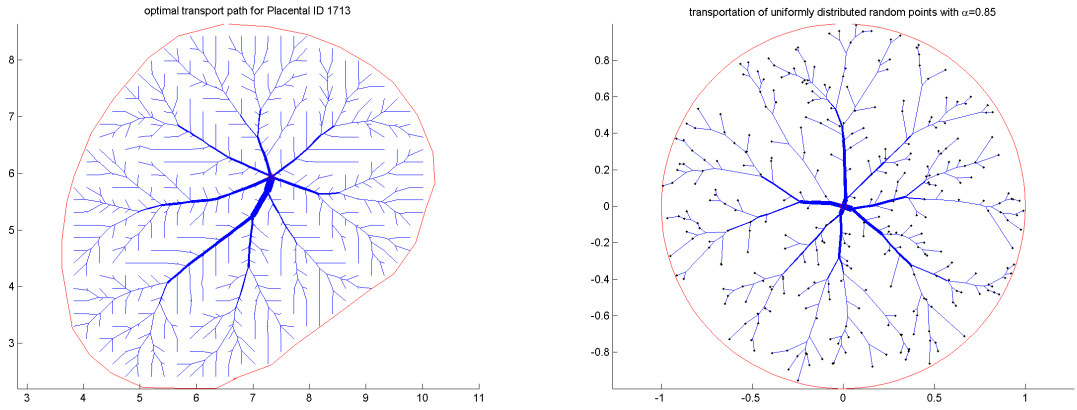

Figure 1: Examples of modeling blood vessels of a placenta by a nearly optimal transport network; The left one is uniformly distributed, while the right one is randomly distributed

For each placenta a total transport cost, based on all measurements, (i),(ii), and (iii), is given by the model. This computed cost is highly correlated with measured birth weight, placenta weight, FPR and the metabolic scaling factor beta. Also a shape factor is given by the model which would be the total transport cost if a placenta were rescaled to have a unit area chorionic plate. This shape factor is also highly correlated with birth weight, and after adjustment for placental weight, is highly correlated with the metabolic scaling factor beta.

Mathematical Immunology and Pathogen Dynamics (SS-MIPD)

Organizers:
Jane Heffernan (York University)

The immune system offers a sophisticated, natural and arguably the most reliable defense mechanism against many infectious diseases. Major advances in knowledge of the organization and function of the immune system and its interactions with infectious pathogens have been made very recently. Yet, significant gaps in knowledge continue to exist. While experimental research has made outstanding contributions by identification and physical characterization of the key components of immune system and their mutual interactions, an understanding of their dynamical behavior as these relate to suppression or persistence of an infection remains limited. Mathematical modelling of the immune system and pathogen dynamics has recently emerged as a major field of study (in the past few decades) and holds great promise in providing new insights into the dynamical processes intrinsic to mechanism and control of infectious diseases. This session includes studies of immune system and pathogen dynamics which contribute to the understanding of immune system protection against infectious diseases, and/or mechanisms and characteristics of pathogens enabling immune escape.

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The known unknowns and the unknown unknowns

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From viral infections we get data. Around the data we build models. Then we squeeze these models to fit through the data... what have we learned? A lot, hopefully. This is a tale of what we have learned by fitting mathematical and computational models to data describing the time course of viral infections within a person (in vivo) or cell culture (in vitro), primarily from influenza infections. But it is also a cautionary tale of the things we missed, hiding in the dark corners of our analyses, from which we can also learn a lot.

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Immunology and the Dynamics of Hepatitis Delta Virus Infection

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Hepatitis Delta Virus (HDV) is a dependent satellite virus of the more common Hepatitis B Virus. HDV encodes only one protein of its own, relying on HBV to supply the additional proteins needed for its replication cycle. The two viral infections interact direct in host cells and indirectly via their influence on the immune system, producing a variety of different dynamical behaviors, ranging from wide oscillations to clearance. In this talk I present a model for the interactions of HBV, HDV and the immune reactions to each. Using this model, I explore how immune factors can influence the course of co-infection, and the consequences this has for patient symptoms and treatment options.

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Dynamics of In-host Malaria Model

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The talk is based on the design and qualitative analysis of a new model for the dynamics between the malaria parasite and the immune system within an infected human host. The model, which incorporates multiple stages of the malaria parasite life-cycle, immune cells and antibodies, is used to assess the potential impact of a future anti-malaria vaccine. Conditions for the existence and asymptotic stability of the associated equilibria are derived. It is shown that a malaria vaccine that reduces the number of *merozoites* and boosts immune response will be quite effective in reducing the concentration of infected red blood cells in the host.

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Linking immunology and epidemiology: dynamics of human rhinovirus in an immune-structured host population

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We develop, present, and analyze an immunoepidemiological model consisting of a mixed system of ordinary differential equations and partial-integrodifferential equations with nonlocal boundary conditions, used to track spread of infection in host structured by a continuously varying immune status. In particular, we focus on the generation of immunity upon infection, the maintenance of immunity within individuals by repeated exposure, and the combined effects of these on population-level transmission. We illustrate the equilibrium distribution of hosts with respect to their immune status for a variety of immune system parameters, such as the strength of the immune response and its waning rate. We highlight features of the system that promote sustained endemic oscillations, and discuss potential implications of oscillations with respect to public health and individual disease severity.

We have extended this framework to study a host population exposed to a diverse community of partially-cross-reactive co-circulating viruses, specifically the human rhinoviruses. With respect to the conditions mentioned above (generation and maintenance of immunity), we discuss implications of infection transmission in immunologically-structured hosts on viral dynamics and diversity. In particular, we focus on the distinction between the major and minor group rhinoviruses, and illustrate how the strength and specificity of the immune response shapes long-term dynamics and viral diversity.

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Modeling within-host dynamics of influenza virus infection

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Influenza, commonly referred to as the flu, is a contagious respiratory illness caused by influenza virus infections. Although most infected subjects with intact immune systems are able to clear the virus without developing serious flu complications, the mechanism underlying viral control is not fully understood. I will address this by reviewing existing models and presenting a new model including immune responses. I will discuss the relative roles of target cell availability, and innate and adaptive immune responses in controlling the virus. I will also discuss combination therapy for influenza.

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The importance of cell-to-cell transmission during the acute stage of HIV infection

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HIV has a number of escape routes when it comes to avoiding the immune system and minimizing the effects of drug therapy, one of the most effective and efficient ways is cell-to-cell transmission. Cell-to-cell transmission protects the virus from the external cellular elements, such as antibody, which would otherwise neutralize it.

Previous models assumed cell-to-cell transmission occurs through mass action mixing or have modelled cell-to-cell transmission with a cellular automaton or agent based model. In epidemiology, the contact network plays a key role in how the disease spreads throughout a population. With cells naturally forming connections between one another a network structure is formed for cell-to-cell transmission to occur, which is overlooked if mass-action mixing is assumed. Cellular automata and agent based models are able to capture and depict realistic within host dynamics; however, due to their extreme complexity it is often difficult to understand the underlying dynamics which are the main cause of the observed results.

We have coupled a meta-population model with a pair approximation model to capture the spatial dynamics and the network structure required for cell-to-cell transmission. The meta-population is separated into two separate regions: the overlying homogeneous system which represents the peripheral blood stream and the underlying spatial system which represents the various lymphatic regions. The objective of our model is to understand the importance of cell-to-cell transmission during the acute stage of HIV infection and the impact cell-to-cell transmission has on the effectiveness of drug therapy.

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A study of recurrent infection in deterministic in-host models

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In latent virus infection, no clinical signs nor detectable infectious cells can be observed during the silent stage of low-level viral replication. However, the virus has not been completely cleared, and recurrent episodes of rapid viral production and release can periodically punctuate relatively long periods in the silent stage. These episodes of recurrent infection are a clinical phenomenon observed in many latent infections [1]; human immunodeficiency virus (HIV), for instance, can be suppressed by highly active antiretroviral therapy (HAART) to below the limit of detection for months or years. Moreover, these long periods of relative quiescence are typically interrupted by unexplained intermittent episodes of viremia above the detectable limit, termed viral blips [2, 3]. To date, many possible explanations for viral blips during HIV infection have been explored mathematically, for example coupled deterministic-stochastic models [4], stochastic models [5], or ODE models with an "on-off" forcing function [3, 2], which can then be explored numerically to simulate viral blips. Although numerical simulation has been invaluable in describing and delineating the behaviour of these models, there is yet very little analytical work exploring the mathematical underpinnings of recurrent infection (or viral blips).

In this talk, we take advantage of dynamical systems theory to reinvestigate a 4-dimensional HIV antioxidant-therapy model [6] which exhibits viral blips, and show that an increasing, saturating infectivity function may contribute to the recurrent behaviour of the model. We then propose four conditions for the existence of viral blips in a deterministic in-host infection model. We use these conditions to derive the simplest (2- and 3-dimensional) infection model which produces viral blips, and determine the complete parameter range for the 3-dimensional model in which blips are possible, using stability analysis. We also use these conditions to demonstrate that low-dimensional in-host models with linear or constant infectivity functions cannot generate viral blips. Further, we find that a 5-dimensional immunological model satisfies the conditions and exhibits recurrent infection even with constant infectivity; thus, an increasing, saturating infectivity is not necessary if the model is sufficiently complex.

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Modeling HIV-1 virus dynamics with both virus-to-cell infection and cell-to-cell transmission

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Direct cell-to-cell transmission of HIV-1 is found to be a more potent and efficient means of virus spread than the virus-to-cell infection mode, but has been overlooked in existing models. In this talks, I will present a mathematical model to include these two modes of viral infection and spread, in which infection age is also incorporated. Analysis shows that the model demonstrates a global threshold dynamics, fully described by the basic reproduction number, which is identified explicitly. The formula for the basic reproduction number turns out to be in the form of superposition relation with the respective basic reproduction numbers due to the two modes separately, not only reveals that the basic reproduction number of a model that neglects either the cell-to-cell spread or virus-to-cell infection is under-evaluated, but also tells precisely by how much it is under-evaluated. We also discuss the implications of our theoretical results which can explain, to some extent, the recent experimental findings by Sigal et al [Nature, 477(2011), 95-98] that cell-to-cell transfer of HIV-1 can lead to multiple infections per cell which may reduce the efficacy of antiretroviral therapy and permit ongoing replication.

Mathematical Models for Nanoscience and Nanotechnology (SS-MMNN)

Organizers:
Z.L. Miskovic (University of Waterloo)
A.H. Majedi (University of Waterloo)

Nanoscience may be defined as confluence of concepts and methods from the traditional areas of Science and Engineering 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 for problems of current interest in Nanoscience and Nanotechnology.

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Substrate Structure Effects on Electrical Properties of Graphene

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Graphene is a new material, which promises to revolutionize the semiconductor industry. The properties of this two dimensional allotrope of carbon has applications in THz radiation receivers, bio-sensors, transistors, ultra-capacitors, and many more devices. Its two dimensional nature gives tremendous sensitivity to its surroundings which increases its applicable nature. However. this sensitivity comes with a price. The material surrounding graphene has to be free of defects and impurities for suitable integration with graphene. In most cases this is impossible, as long-range scattering defects are present in all materials. Charge impurities in the substrate, which cause long-range scattering in the graphene sheet, affect the conductivity and the distribution of charge carriers in graphene.

It is theorized that charge impurities in the substrate cause nonzero conductivity in graphene even when there are no charge carriers present in the graphene sheet [1]. This has been attributed to the impurities in the substrate which cause the formation of electron-hole puddles in graphene [2]. The electron-hole puddles exhibit length correlation which have been observed experimentally [3] .There is a slight asymmetry in the conductivity of graphene around the Dirac point for electron and hole doping. Cause of this affect has still not been resolved but we have evidence to believe it comes from dipole moments associated with impurities.

In our work we will show how a finite size of the dielectric substrate could enhance the minimum conductivity of graphene and how dipole impurities in the substrate could cause an asymmetric conductivity around the Dirac point. Also we will show how correlated impurities in the substrate give rise to electron-hole puddle formation in graphene. For this we will use a two dimensional hard-disk model for the spatial correlation among the impurities. All these results will be derived using semi-classical electron transport theory and statistical mechanics. We will compare our theoretical results of the conductivity and potential correlation in the graphene sheet with recent experimental results.

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Effect of Microwave and Terahertz Radiation on Superconducting Nanowires

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In this talk, we will discuss the effect of the Microwave and Terahertz radiation on Superconducting Nanowires. Theoretical and Experimental results on the on-chip generation and detection of Microwave and Terahertz radiation will be presented. We will also argue that the radiation from adjacent elements in a multi-element Superconducting Nanowire Single Photon Detectors (SNSPD) can decrease the quantum efficiency in photon detection. We will compare our results with the previous work on multi-element SNSDPs, where they observed negligible effect due to adjacent elements (see Ref [1]).

Reference

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Spectra of Few-body complexes in Quantum Dot Molecules

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Entanglement is the most peculiar yet realizable manifestation of quantum physics. During the past decade, low-dimensional quantum confined systems have shown promising features toward actualizing on-demand sources of entangled particles. However, in order to observe such a delicate phenomenon, highest control in initialization, manipulation and readout of the quantum states is necessary. In this context, high fidelity entanglement between spin and photon, or between flying photon pairs, has not been achieved yet.

The ground state excitonic transitions in quantum dots (QDs) are known as potential sources of polarization-entangled photons [1]. In this work, we analyse the few-particle excitonic complexes localized in a double quantum dot. We particularly demonstrate how in QD molecules (QDM) the formation of different configurations of complexes relies on few-body interactions when the single particles are Coulomb-correlated. Our results explain how the hybridized states in QDM may provide energy coincidence between different spectral features, which is the primary requisite for generating entangled photon states.

Our calculations comprise almost all the relevant effects influencing the energy fine structure of a typical QD, including strain, piezoelectricity, spin-orbit interaction and band mixing along with exchange and correlation energies [2]. To account for the few-body correlations we utilize Configuration Interaction (CI) method. Our CI model benefits from the underlying band structure and the single particle orbitals solved via multi-band *k.p* theory developed for III-V materials in zinc-blende phase [3].

In the final step, we examine how electric and magnetic fields parallel and perpendicular to the QD quantization axis could tailor the tunnelling matrix element and energy fine structure of favourable excitonic complexes in QDM. These external fields, simultaneously applied on the QDM, provide controllability of spectral features with hight energy resolution.

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An integral equation solver for the simulation of two-dimensional metallic nanoplasmonics

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Nanoplasmonics forms a major part of the field of nanophotonics, which explores how electromagnetic fields can be confined over dimensions on the order of or smaller than the wavelength. Initiated in 1902 by R.W. Wood [1] with the discovery of grating anomalies, this phenomenon has attracted significant attention over the last hundred years [1, 2, 3]. Mie in 1908 gave a mathematical description of light scattering from spherical particles of sizes comparable to the wavelength [2], describing an effect that will come to be known as localized surface plasmons in the context of nanoplasmonics. It is based on interaction processes between electromagnetic radiation and conduction electrons at metallic interfaces or in small metallic nanostructures, leading to an enhanced optical near-field of sub-wavelength dimension.

All of the phenomena mentioned above are based entirely on classical electromagnetics, and thus can be mathematically described by Maxwell's equations. Here in this talk, integral-equation formulation will be given for an infinitely periodic metal surface whose period d is on the nanometer scale. The metal is assumed to extend infinitely below the surface, while a dielectric material extends infinitely above the surface.

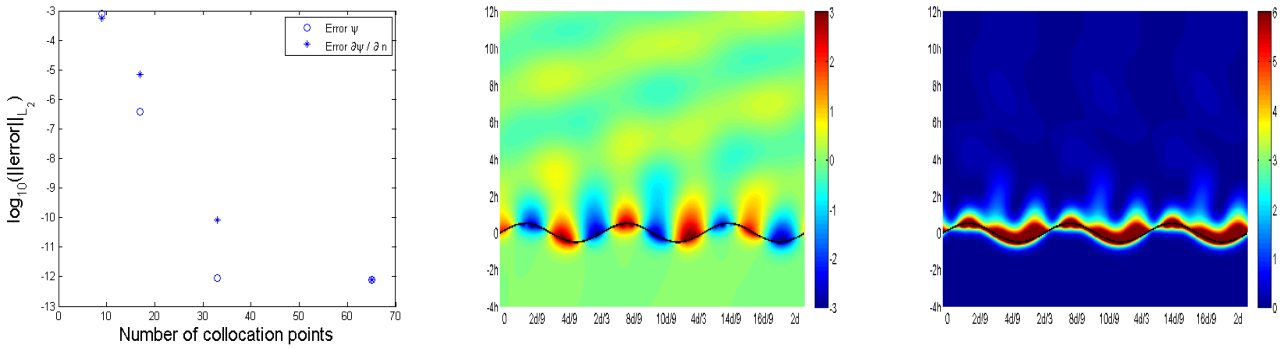

Figure 1: Here we provide numerical results for the sinusoidal gold grating for the incidence angle $\theta = 29^o$. Left: The error on a logarithmic scale for the convergence of the total field and its normal derivative on the surface of the grating. Middle: Real part Right: intensity of the scattered field above and below of the grating.

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Tackling Surface Roughness in Graphene Plasmonics

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Plasmons are collective oscillations of electron density, and they have found much use in modern electronics and sensing because of their confinement of electromagnetic radiation to dimensions smaller than their wavelength. Graphene, a two-dimensional carbon lattice, has the ability to tune and adjust these plasmons with a great deal of versatility. Combining the two has led to the field of *graphene plasmonics* (Ref. [1]). The effect of surface roughness in both the graphene and its substrate is essential to achieving the fine tuning required of these plasmons and is the subject of this research.

By modelling the substrate as a randomly rough surface with graphene on top, the graphene can be treated with a two-dimensional Vlasov equation. This problem can be rephrased in terms of a random operator equation, and projection operator methods can be used to see how the plasmon frequency (given by charge carriers in the substrate's dielectric constant) depends on roughness parameters like mean square deviation, transverse correlation length and the height of graphene above the substrate. The graphene acts by inducing an image potential in the substrate, hence affecting its own plasmon modes (Ref. [2]).

Preliminary results show roughness yields a small increase in the plasmon frequency, with changing frequencies depending on the degree of roughness in both the graphene (due to local curvature of its surface) and the substrate (natural roughness of metals and insulators). Its small effect can help optical circuit designers optimize the type of surface needed to subtend graphene, and to intentionally have rougher surfaces in order to induce higher frequency plasmons.

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Piezo-electromechanical effects in embedded nanowire superlattices

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Modifications of the band diagram of semiconductor nanostructures by utilizing current state of the art in nanotechnology are of great interest fto photonics, light emitting diodes and other optoelectronic devices. In this contribution, we investigate the influence of piezo-electromechanical effects on the band structures of electron (hole) states of GaN nanowire supperlattices (NWSLs) embedded into an AlN matrix. We develop a multiscale multiphysics simulation strategy based on the Finite Element Method and solve the coupled strain dependent 8-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian model in 3D Cartesian coordinates. We focus our study on the barrier localization of electron (hole) states of wurtzite AlN/GaN SLs structure. Several parameters such as lattice mismatch, piezoelectric fields, valence and conduction band offsets at the heterojunction of $Al_xGa_{1-x}N/GaN$ SLs can be varied as a function of the Al mole fraction. When the band offsets at the heterojunction of $Al_xGa_{1-x}N/GaN$ are very small and the influence of the electromechanical effects can be minimized, then the barrier material can no longer be treated as an infinite potential well. In this situation, it is possible to visualize the penetration of the Bloch wave function into the barrier material that provides a quantitative estimation of the critical radius in such NWSLs. In this case, the NWSLs can act as an inversion layer.

Representative plots of probability distributions of electrons and holes are shown in Fig. 1(a). Since, we do not include the piezo-electromechanical effects in the first instance (1(a,b)), we find that the electron and hole wavefunctions are localized at the center of the nanowire SLs. Next, we reduce the Al mole fraction in $Al_xGa_{1-x}N/GaN$ NWSLs which leads to the reduction in the band offsets. In this situation, the influence of piezo-electromechanical effects is minimized and the penetration of electron (hole) wavefunctions can be seen to the barrier materials. Thus the barrier materials act an inversion layer. These results are shown in Fig. 1 (c).

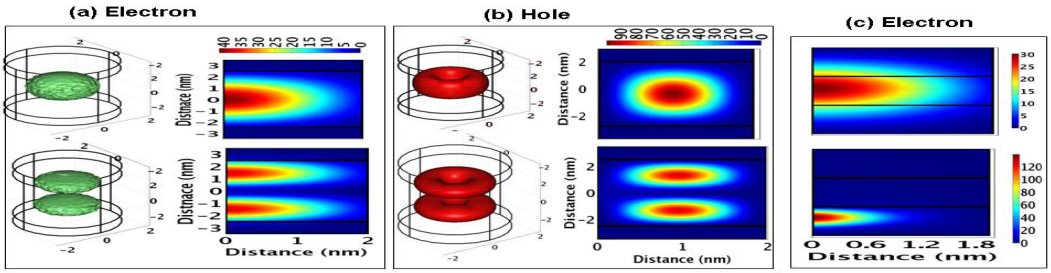

Figure 1: Modeling of the distributions of electron and hole densities in AlN/GaN/AlN superlattices. Upper panel shows the ground state wavefunctions and lower panel shows the first excited state wavefunctions.

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Effects of finite ion size and dielectric saturation of water in electrolytically top-gated graphene

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Interactions of graphene with an electrolyte are cardinal to its applications to chemical and biological sensors, where graphene operates in the configuration of a field-effect-transistor (FET) with its surface exposed to a liquid containing mobile ions, whereas the applied gate potential controls the current through graphene. While carbon nanotubes have been thoroughly investigated in this context, studies on utilizing graphene as biochemical sensor have only recently begun to appear. The top gating of graphene FETs with liquid electrolyte also exhibits numerous merits for nano-electronic applications in comparison to the conventional back gating with a metallic electrode.

Recently, we have modeled [1] electrolytically top-gated graphene taking into consideration nonlinear polarization of graphene and the ion crowding effect [2] in the nearby electrolyte due to steric effects, i.e., the effects of finite size of dissolved ions. In that regime, we used a series combination of the capacitance of double layer in electrolyte and quantum capacitance of graphene [3]. Because such applications are dealing with relatively large potential drops across double layer and correspondingly large charge carrier densities in graphene, it is crucial to also take into account dielectric saturation of the solvent (in our case water) in strong electric field near the surface of graphene. In addition, we want to retain the steric effects in our model to be able to describe situations with high ion concentrations. To describe those effects we use two models: Booth model for dielectric saturation [4] and Bikerman model for steric effects [5]. Hence, we bring forth an improved model by blending steric effects and dielectric saturation of water and incorporating them into modified Poisson-Boltzmann equation.

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Multitaper Spectrum Estimation, Prolate Spheroidal Wave Functions, Quadratic-Inverse, and Related Problems (SS-MSEPSW)

Organizers:
Wesley Burr (Queen's University)
Charlotte Haley (Queen's University)
David J. Thomson (Queen's University)

Since its invention in 1982, the multitaper spectrum estimation tool has become an integral part of signal processing. The underlying theory of the multitaper relies heavily on the Prolate Spheroidal Wave Functions and Sequences (shortened to prolates), as explored by Slepian, Pollak and Landau. This mini-symposium is intended to serve two purposes. The first is to explore the development and application of the multitaper tool to diverse scientific fields, especially those involving nonlinear and nonstationary data sets. The second is to examine current research on prolates, especially (but not limited to) computational and algorithmic developments. Our hope is that the cross-fertilization between these two traditionally unrelated fields will spark new applications and research opportunities. We especially welcome talks on the theory and sampling properties of prolate-based and Quadratic-Inverse-type estimators.

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Discrete Prolate Spheroidal Sequences as Filters in Generalized Additive Models

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The Air Health Indicator is a joint Health Canada / Environment Canada initiative that seeks to model the Canadian national population health risk due to short-term (acute) effects of air pollution. The commonly accepted model in the field [1, 2] uses cubic spline-based temporal smoothers embedded in Generalized Additive Models [3] to account for seasonal and long-term variations in the response. From a spectral point of view, it is natural to think of these smooth, long-term variations as low-frequency components, and the temporal smoother as a digital filter.

Examining the frequency response of the filters typically used, we show that the performance leaves much to be desired. Adapting the discrete prolate spheroidal sequences [4] as filters, taking inspiration from their similar use in the *multitaper method* [5], we are able to significantly improve the frequency response of the smoother. We conclude with a discussion of the implications of this change for the desired outcome of estimating population health risk due to acute air pollution, and the computational concerns in using this algorithm.

This work was partially supported by Health Canada through contract #4500250926.

Key words: population health risk, Generalized Additive Models, smoothers, filters, prolates, multitaper

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Signal and Spectral Estimation on a Sphere

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We address the problem of estimating the spherical-harmonic coefficients (Problem I), and also the isotropic power spectrum (Problem II), of a scalar (and if time permits, also of a vectorial) signal from noise-contaminated data on a region of the unit sphere. As to Problem I, the estimation of potential fields such as the gravitational or magnetic potential at the surface of a spherical planet from noisy observations taken at an altitude over an incomplete portion of the globe is a classic example of an ill-posed inverse problem. We show that this potential-field estimation problem has deep-seated connections to Slepian's spatiospectral localization problem which seeks bandlimited spherical functions whose energy is optimally concentrated in some closed portion of the unit sphere. This allows us to formulate an alternative solution to the traditional damped least-squares spherical harmonic approach in geodesy, whereby the source field is now expanded in a truncated Slepian function basis set. We discuss the relative performance of both methods with regard to standard statistical measures such as bias, variance and mean squared error, and pay special attention to the algorithmic efficiency of computing the Slepian functions on the region complementary to the axisymmetric polar gap characteristic of satellite surveys. The ease, speed, and accuracy of our method make the use of spherical Slepian functions in earth and planetary geodesy practical. As to Problem II, three different methods of spectral estimation are considered: (i) the spherical analogue of the one-dimensional (1-D) periodogram, (ii) the maximum-likelihood method, and (iii) a spherical analogue of the 1-D multitaper method. The periodogram exhibits strong spectral leakage, especially for small regions of area $A \ll 4\pi$, and is generally unsuitable for spherical spectral analysis applications, just as it is in 1-D. The maximum-likelihood method is particularly useful in the case of nearly-whole-sphere coverage, $A \approx 4\pi$, and has been widely used in cosmology to estimate the spectrum of the cosmic microwave background radiation from spacecraft observations. The spherical multitaper method affords easy control over the fundamental trade-off between spectral resolution and variance, and is easily implemented regardless of the region size, requiring neither non-linear iteration nor large-scale matrix inversion. As a result, the method is ideally suited for most applications in geophysics, geodesy or planetary science, where the objective is to obtain a spatially localized estimate of the spectrum of a signal from noisy data within a pre-selected and typically small region.

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Analysis of Multitaper Covariance and Autoregressive Spectral Estimates

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A seamless and smooth transition from nonparametric multitaper (MT) spectral estimation (SE) to autoregressive (AR) parametrization is made possible via autocorrelation estimates from multitapered data [1]. The autocorrelation estimates were shown [2] to be more compact and of lower variance than ordinary autocorrelation estimates. We derive the Cramer-Rao bounds of the autocorrelation estimates and compare them to the Capon estimation of the same [3]. The paper also analyses the effect of the MT covariance estimates on MTAR spectral estimates and provide examples from simulated test data as well as speech data.

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Multitaper Smoothed Minimum Statistics Noise Power Estimation

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Speech communication devices and digital hearing aids must perform in the presence of high levels of ambient noise. Speech enhancement is a denoising process where Wiener-like filters are developed that require the estimation of the background noise spectrum from an additive combination of speech and noise. To follow statistical variations over time, the processes must be performed over short and overlapping frames of data resulting in time varying filters and spectra. Tracking of non-stationary noise is a difficult task for single-microphone systems because of the shared characteristics of some speech segments and noise. The minimum statistics approach to noise power estimation relies on a biased estimate of the noise floor at a given frequency as the spectral minimum of a number of consecutive frames. The spectral sequence is smoothed by a recursive filter with time and frequency dependent parameters. The resulting estimate is biased toward lower values. The bias depends on the variance of the smoothed power and the smoothing filter coefficients which are empirically chosen.

We propose an alternative formulation to tracking the noise power that replaces the smoothing filter coefficients with MultiTaper Autoregressive filter coefficients. The resulting filter coefficients are derived from the data and show superior tracking of the time-variation of the spectra. The smoothed minimum spectrum output has low variance and low bias.

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Jackknifing Multitaper Autocorrelation Estimates

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In this paper, we investigate the multitaper (MT) autocorrelation function (acf) estimator, which is defined as the inverse Fourier transform of the MT spectrum estimator. McWhorter and Scharf [1] have shown that estimates of the acf constructed using multiple windows possess three desirable properties which the conventional (Bartlett) acf does not, namely that they are (i) quadratic in the data (ii) nonnegative definite, and they have (iii) modulation covariance. It is also known that in comparison with the Bartlett acf, the "ringing sequence", or spectrum of the sequence of errors in the estimate of the acf, the MT estimator of autocorrelation damps more quickly to zero [2].

Various authors have attempted to quantify the improvement of the MT acf over the Bartlett estimate, e.g. [1, 3, 4]. Here, we show that because individual *eigencorrelation* estimates (acf estimates constructed with a single Slepian taper) are approximately uncorrelated (due to the orthogonality properties of the Slepian tapers) it is possible to construct a jackknifed estimate of acf variance. By means of a Fisher's Z transformation, the correlations become approximately normal, and thus can be used to calculate confidence intervals (CIs). The CIs can be carried through to the partial acf, and are useful to obtain error bounds on parametric spectra and prewhitening filters.

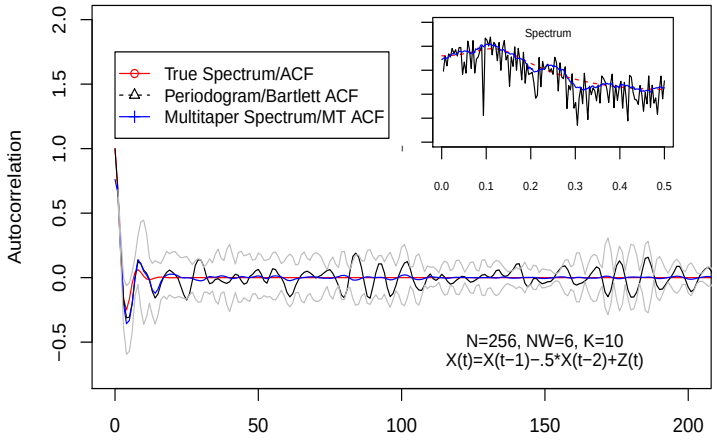

Figure 1: A 256-sample AR(2) example in which the Bartlett and MT autocovariances and spectra are plotted along with the MT CI.

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Paleoclimate time scale estimation using multitaper spectral methods

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Geology is replete with long sedimentary sequences that were deposited in response to paleoclimate change. It is rare, however, that an adequate time scale is in attendance for accurate assessment of the recorded paleoclimate. Other problems include: variable sediment accumulation (time scale distortion); non-stationary climate signals; non-linear climate signals; noise interference; biased and/or truncated data sampling. Some frequency bands are associated with deterministic signals, notably Milankovitch cycles with line frequencies in the 10^{-4} to 10^{-6}/year band. This provides the singular opportunity to exploit Milankovitch cycles for tuning paleoclimate records. This tuning strategy has been used since the 1970's [1], but has often been criticized as subjective and prone to circular reasoning [2, 3]. This has motivated the development of objective approaches for estimating paleoclimate time scales, in which multitaper spectral methods have played a transformational role.

The simplest of these new approaches is "minimal tuning." The spectrum of a paleoclimatic signal is examined for significant lines, from which one is assumed to represent a Milankovitch term, e.g., the obliquity cycle. The line is examined and corrected for deviations from its expected frequency in an evolutionary analysis along the sequence. Application of multitaper harmonic analysis is central to the procedure. However, minimal tuning still contains a significant element of subjectivity. Thus, the "average spectral misfit (ASM)" procedure was developed to remove all decision-making from the tuning [4]. ASM relies on multitaper harmonic analysis to identify recorded lines, which are then statistically tested against model Milankovitch lines assuming different sediment accumulation rates. If a solution can be found, then other aspects about the paleoclimate record can be addressed, e.g., non-linearities or noise attributes. We apply these techniques to selected paleoclimate records of different geologic ages, and discuss pitfalls and future improvements.

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Estimating evoked brain connectivity with discrete prolate spheroidal stimulation

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Brain network connectivity has been inferred using passive measurements of ongoing activity across recording sites. With this paradigm it is difficult to determine how activity in one region induces activity in another. To obviate this issue, active brain stimulation has been employed, recently using a combination of adaptive stimulation and Bayesian network estimation [1, 2]. In these previous works, to separate the influence of one brain region upon another, only a single brain region is stimulated prior to each recording epoch. In the current, preliminary work, multiple brain regions are stimulated simultaneously with modulated discrete prolate spheroidal sequences of differing orders. By exploiting newly discovered and approximate orthogonality relations, the relative influence of each stimulated brain region upon every other brain region is separated – facilitating the use of more flexible cost functions for neural network discovery, tracking and control.

The talk begins with the description and characterization of the further orthogonality relations of the discrete prolate spheroidal sequences. Following a brief discussion of sequential, adaptive, neural evoked connectivity estimation, the proposed multi-region stimulation strategy is presented. The talk ends with a verification of the methodology on a Wilson-Cowan mean-field model of neural activity.

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Spectral Coherence Evidence for Oceanic Control of Interannual Carbon Cycle Feedbacks

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Large-scale carbon-cycle feedbacks within Earth's climate system can be inferred from the statistical correlation of atmospheric CO^2 and other climate observations. These statistical relationships can serve as validation targets for global carbon-cycle models. Multiple-taper coherence between atmospheric CO^2 measured at Mauna Loa, Hawaii, and Hadley Centre global-average temperatures changed in the late 20th century at interannual frequencies, from a 6-month time lag to a 90^o phase lag that scaled CO^2 fluctuations to a time-integral of the global-average temperature anomaly. Wavelet coherence estimates argue that this change occurred with a recognized ocean-circulation climate transition during the late 1970s. The CO^2-coherence phase differs with the source of the temperature measurement, in a way that indicates a close relationship with sea-surface temperature (SST). The latitude dependence of the leading principal component of interannual GLOBALVIEW CO^2- variability suggests a terrestrial influence that is not linked to land temperatures. The correlation of terrestrial CO^2 variability with SST suggests a connection via moisture transport rather than with local warmth.

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Multitaper Spectrum Estimation and Quadratic-Inverse Theory: from Conception to Present

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Multitaper spectrum estimation refers to a set of methods for estimating the power spectrum and, by extension, autocorrelations, coherences, and similar statistical descriptive functions of a time series by using several tapers on each data segment before taking Fourier transforms [1, 2]. The data tapers are usually *discrete prolate spheroidal sequences* [3], now called *Slepian sequences*, the eigenvectors of the finite Fourier transform. In this talk I review the development of these methods, including history, and describe some applications to climate.

The second part applies *Quadratic–inverse* theory to the solar wind. QI [4, 5] extends multitapering to orthogonal quadratic forms in the eigencoefficients that describe, *e.g.*, functions such as the time derivative of a spectrum. The interplanetary magnetic field is nonstationary with a time–varying spectral index (the slope on a log–log plot). One needs approximately three–hour blocks to estimate the spectra and 16–minute time resolution, so resolving this nonstationarity pushes resolution to its limits. Given the series of spectral indices, much of the variations is due to solar gravity–modes.

Key words: multitaper, quadratic–inverse, turbulence, space physics, solar wind

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Localized Band-Limited Representation and Robust Interpolative Image Manipulation

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With the rapid development of imaging devices and ever increasing computational power, a wide variety of interesting image analysis problems have arisen in fields ranging from medicine, chemistry, geophysics, satellite imagery and remote sensing to digital photography. Whether for the purpose of segmenting cancerous cells from healthy ones via hyper-spectral imaging, or reconstructing a 3-d model of proteins from 2-d slices, (features of) objects in an image often need to be modeled, detected, extracted, enlarged, and cataloged. The effectiveness of the approaches generally depends upon the underlying mathematical model used for representing the images.

Although images are seldom truly band-limited (i.e. have compactly supported Fourier transforms), they are generally considered "piece-wise smooth" and are frequently modeled *locally* as such by polynomials and trigonometric functions. In particular, image representation and band-limited functions are no strangers to one another. Indeed, DCT transform is part of the popular image format JPEG; many other algorithms in image processing (filtering, encoding, edge detection, texture analysis, etc) use Fourier analysis as a basic tool.

When images satisfy the periodic boundary condition (that is the boundary pixels match with one another when the image is periodically tiled across the whole plane), or can be approximated by one that does, Fourier's methods give very satisfactory results. However, it is well-known that band-limited methods based upon trigonometric functions encounter difficulties with images that do not satisfy the periodic boundary condition.

Under certain conditions, it can be shown that Prolate Spheroidal Wave Functions (PSWFs), a classical special functions that are localized in both spatial and frequency domains a natural choice. We present in this paper a novel image modeling framework based on the PSWFs. We show examples of the Prolate functions, as well as methods for the expansion of images in this basis. Examples of interpolative image manipulations based on this representation will be presented.

New Computational Techniques for Applied Problems in Science and Engineering (SS-NCTAP)

Organizers:
Ludwig Kohaupt (Beuth University of Technology Berlin), Yan Wu (Georgia Southern University)

In today's world, computational techniques play an ever growing role in science and engineering. This is reflected by new notations such as, e.g., Computational Chemistry or Computational Engineering. New disciplines like these are driven by the need to model and analyze systems already in the concept phase before experiments can be made since this procedure can save a lot of time and money, that is, for economic reasons. This special session is therefore devoted to problems in science and engineering that could be useful in real-world applications. Both analysis and modeling aspects are considered.

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Structure-Preserving Simulation of Mechanical Systems

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In mechanics, it may be beneficial to make velocity substitutions that are not tied directly to the configuration coordinates. This use of non-coordinate frames often simplifies the equations of motion and provides insight into systems with symmetries and/or velocity constraints [1, 2]. The development of numerical integrators for the simulation of such systems is of interest [3]. In particular, variational integrators are algorithms that preserve key mechanical structures and are known to perform well in long term numerical simulations of mechanical systems [4]. We will present recent findings in the development of such integrators using the aforementioned non-coordinate frames along with simulations that illustrate their usefulness.

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Matrices of Green's Type for Sets of Laplace Equations Posed on Joint Surfaces of Revolution Weakened with Apertures

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Well-posed boundary-value problems stated in multiply-connected regions are targeted for some sets of two-dimensional Laplace equations written in geographical coordinates on joint surfaces of revolution. These are problems that adequately simulate potential fields generated by point sources in joint perforated thin shell structures comprised of fragments of different geometry. Each fragment in the assembly is made of an individual homogeneous isotropic conductive material. The ideal thermal contact is assumed through the fragments interface line.

A semi-analytical approach is developed to accurately compute solutions of targeted boundary-value problems. The approach is based on Green's function modification of the classical boundary integral equation method. This reduces the problems under consideration to some functional (of integral type) equations.

The Green's-function-based numerical methods have, in nowadays, been proven extremely efficient in solving a wide range of ordinary and partial differential equations that arise in engineering and natural sciences. It is worth noting that coefficients of the governing differential equations appear discontinuous in the targeted boundary-value problems. The discontinuity occurs at the interface lines where the surface geometry changes, making it impossible for direct implementation of the Green's function formalism. This puts us in a position to implement instead the matrix of Green's type concept as introduced in [1]. The elements of the required matrices of Green's type are analytically obtained in a closed computer-friendly form, allowing us to efficiently solve the targeted class of problems.

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Solution of Wiener-Hopf and Fredholm integral equations by fast Hilbert and Fourier transforms

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We present efficient numerical methods based on the fast Fourier transform (FFT) to solve the linear integral equation of convolution type with constant limits of integration

$$\lambda f(x) - \int_a^b k(x-x')f(x')dx' = g(x), \quad x \in (a,b),$$

where $f(x)$ is the unknown function, $k(x)$ is a given kernel, and $g(x)$ is a given so-called forcing function. The domain of $f(x)$ and $g(x)$ is (a,b), the domain of $k(x)$ is $(a-b,b-a)$; the endpoints can be included if they are finite. If $a = -\infty$ or $b = +\infty$ Eq. (1) is called a Wiener-Hopf equation [1, 2, 3, 4, 5]; if both integration limits are finite, it is called a Fredholm equation [4, 6] or a Wiener-Hopf equation on a finite interval [7]. If $\lambda = 0$ it is an equation of the first kind; if $\lambda \neq 0$ it is an equation of the second kind. Historically these equations arose in physics, e.g. to describe diffraction in the presence of an impenetrable wedge or of planar waveguides [8], but also for problems in crystal growth, fracture mechanics, flow mechanics, geophysics, and diffusion [5]. More recently these equations have become of interest in finance to price discretely monitored path-dependent options as barrier, first-touch, and lookback or hindsight options [9, 10, 11]. We extend and improve a FFT-based method for the Wiener-Hopf equation due to Henery [12], expressing it in terms of the Hilbert transform, and computing the latter in a more sophisticated way with sinc functions [13]. We then generalize our method to the Fredholm equation reformulating it as two coupled equations [2, 7, 10] and solving them iteratively. We provide numerical tests and open-source code.

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Integration of Inventory Decisions and Supplier Selection to Optimum Design of Cellular Manufactruing Systems: A Stochastic Solution Space

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In this research, we aim to design cellular manufacturing systems (CMSs) which optimize the performance of manufacturing systems subject to optimization of inventory and supplier selection decisions. In this study, it is assumed that the demand of each product is stochastic and is explained by a discrete set of scenarios. This mathematical model tries to optimize the expected inventory cost and also the subcontracting cost arisen by suppliers for exceptional operations. The initial version of the model will be nonlineare because of integartion strategic decision (cell formation) and tactical / operational decisions (inventory and supplier selection). So, this model will be reduced to linear form by linearization techniques. In any manufacturing environment, supply chain network structures have a vital role in order to produce products. A manufacturer can decide whether the operations are completed within the system or they have to be outsourced to the suppliers in a supply chain network. Thus, suppliers can affect on the characteristics of operation processes which are not completed inside the system. Once there are multi suppliers for each product, decision maker have to select the best one for subcontracting products based on the different criterions such as transportation, inventory policies and location of warehouses. By this way, the structure of supply chain network will be optimized through the mathematical model.

In this study, since the demand is uncertain, stochastic optimization thechnique will be applied. In the structure of any stochastic programming (SP) problem, one must decide which decision variables are first stage and which are second stage; in other words, which variables must be determined first and which may be determined after the uncertainty has been realized. So, in a stochastic CMS problem which we are interested, CF decisions must be made now (design variable), before it is known which scenario will come to pass, while inventory and supplied selection decisions are determined in future after uncertainty has been realized (control variable). Also, we propose a parallel structured solution approach to solve introduced stochastic and nonlinear model in large-scale problems, efficiently. The proposed algorithm involves new combination of genetic algorithm (GA) and simulated annealing (SA) where both algorithms try to find sub optimal solution in a parallel structure considering exchanging data and information between each other. In addition, Fig 1 illustrates the conceptual framework of our method. In this process, GA and SA algorithms attempt to obtain sub optimal solution and also share their information about the best solution, simultaneously. In this way, each algorithm sends information about sub optimal solution to the other algorithm through some designed information channels. Finally, effectiveness of the method will be validated through executing statistical hypothesis test via a heuristic benchmark procedure.

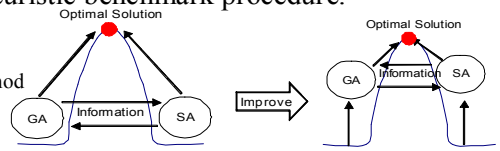

Figure 1: The Conceptual framework of the proposed solution method

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Monte Carlo Study of the Area Estimation Improvement by the Pairwise Comparisons

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Random but visually nice shapes are often needed for cognitive experiments and processes. They are generated from random polygons by applying Gaussian blur with a set threshold in order to transform pixels to black and white from different shades of gray. It produces shapes which are not "sharp" or otherwise hard to estimate for the area thus we call them placated shapes. They are fit to test cognitive processes, such as estimation improvement by pairwise comparisons. Placated shapes can be also used in computer games or in software testing. No one really knows what a "nice" shape is. However, we can recognize a nice shape once we see it. The results of testing randomly generated bars for the length (1D case) were published in [1, 2] as the first such study ever conducted. The length estimation error went down from approximately 15% (by direct method) to approximately 5% by the pairwise comparisons method. It is harder to do with the 2D case since shapes such as circle or square have proportionality, hence placated shapes must be used, but their production is non-trivial. An experiment was designed and published in [4] where random but equal in area shapes were used. The shapes used were manually created [3]. Respondents were tricked into comparing random but equal shapes (according to the area), without knowing that all shapes had identical area, by a cognitive experiment designed in [4]. Only a few such respondents correctly guessed the equality. This study extends the 2D case to random area like shapes in Fig. 1. The generated shapes are subject to selection from a set of 72 (90% accuracy requires at least 68 objects so a 9 by 8 table is used for displaying images) shapes according to the taste of the tester. The user can then compare and estimate the area of the selected shapes. Statistical analysis is conducted by replicating the tests used in [1, 2].

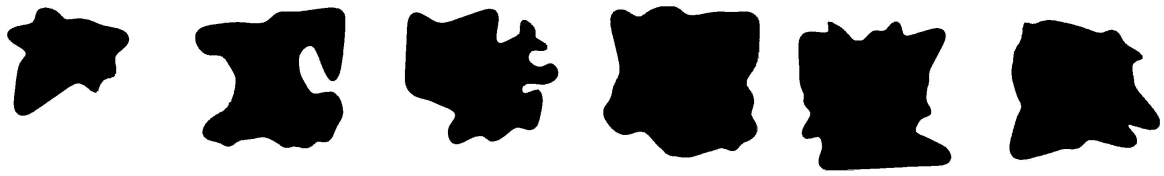

Figure 1: Randomly generated shapes with unequal area size

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Iterative analytic approximation to nonlinear convection dominated systems

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In this paper we are interested in the analytic approximation of nonlinear convection dominated systems of mathematical physics. Solutions of such systems, contaminated by a small parameter, often show sharp boundary and interior layers. The problem becomes still more complex as the equation under consideration is having nonlinearity together with small dissipation. Then, shock waves appear alongside boundary layers. To approximate the multi-scale solution of convection dominated problems, we present and analyze an iterative analytic method based on a Lagrange multiplier technique. The Lagrange multiplier is obtained optimally, in a general setting, using variational theory and Liouville-Green transforms. The idea of the paper is to overcome the well known difficulties associated with the numerical methods. Examples, with quadratic nonlinear convection term and quasi-linear terms, are taken into account to show the effectiveness and accuracy of the present approach. It is observed that the method is straightforward, highly accurate and brief. Moreover, it can also be functional to other nonlinear evolution equations of mathematical physics

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On the vibration-suppression property and monotonicity behavior of a special weighted norm for dynamical systems $\dot{x} = Ax$, $x(t_0) = x_0$

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In an earlier paper, the author formed a positive definite matrix R as the sum of positive semi-definite matrices that are eigenmatrices of a matrix eigenproblem associated with the Lyapunov matrix equation. This positive definite matrix R was then used to define the weighted norm $\|\cdot\|_R$ in C^n which led to new two-sided bounds on the solution of the initial value problem $\dot{x} = Ax$, $x(t_0) = x_0$, in any vector norm $\|\cdot\|$. In the present talk, the quantity $\|x(t)\|_R$ itself is analyzed showing that the solution $x(t)$ in the weighted norm $\|x(t)\|_R$ suppresses the vibration behavior inherent to $x(t)$. This new sight at the norm $\|x(t)\|_R$ may be of considerable practical use in technical dynamical systems. As a direct important application in engineering, the quantity $\|x(t)\|_R$ may be used as a measure to assess the damping behavior of the studied free dynamical system since the vibratory part is absent. Moreover, it is shown that $\|x(t)\|_R$ is monotonically decreasing for sufficiently large t if matrix A is asymptotically stable. Thus, as a further application, a two-sided estimate of the form $c_0\,|D_+\|x(t)\|_R| \le \|\dot{x}(t)\|_R \le c_1\,|D_+\|x(t)\|_R|$ can be derived, which is shown to be invalid for the norm $\|\cdot\|_2$. This result is also of interest on its own. The obtained findings are underpinned by a numerical example and illustrated by graphs.

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Interactive computational search strategy of periodic solutions in an essentially nonlinear dynamics

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We consider essentially nonlinear autonomous and non-autonomous dynamic systems based on ordinary differential equations. In such systems, at the same parameters of the system and forcing can exist different stable and unstable solutions of different periods. In addition, along with the ordered movements, known the existence a strange attractor. In such circumstances, the search for periodic solutions and their stability analysis is not a trivial problem.

For finding periodic solutions of the dynamical systems we offer an interactive computer algorithm based on finding the initial conditions corresponding to the periodic solution with the possibility interactive intervention and operational control by computing process.

We demonstrate the algorithm and various numerical examples of finding new and complex stable and unstable periodic solutions in strongly nonlinear dynamical systems with one and two degrees of freedom. We also consider the examples of the bifurcation of periodic solutions on the boundary of the strange attractor, the mutual influence of oscillations in multidimensional nonlinear dynamic systems.

For example, for non-autonomous dynamical system of the form (1) with N = 1 found new solutions with different periods and strange attractor, with N = 2 were observed as the mutual influence of different forms of oscillations (Fig. 1).

$$\ddot{x}_j(t) + j^2(k^2 j^2 + D)x_j(t) + x_j(t)\frac{j^2}{4}\left(\sum_{m=1}^{N} m^2 x_m^2(t)\right) + \\ + \delta_1 \dot{x}_j(t) = Q_j(t), Q_j(t) = Q_j(t+T),\ j = 1,2,...,N \qquad (1)$$

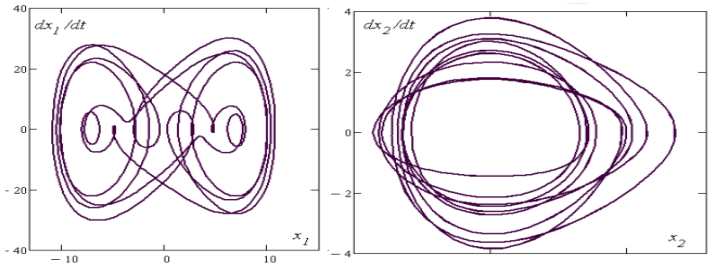

Figure 1: The phase trajectories of 3T-periodic stable solutions of system (1).

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Exploring Stochasticity and Imprecise Knowledge Based on Linear Inequality Constraints

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It is often desirable to find the range of possible values for some real valued function, g, of a set of parameters, $\mathbf{p}$. Here we consider the case where prior knowledge about a finite number of k parameters, $\mathbf{p} = (p_1, \ldots, p_k)$, which characterize a stochastic model or process can be expressed through a set of linear inequalities. For each given value of $\mathbf{p}$, we intend to calculate

$$\mathbf{a} = g(\mathbf{p}) \tag{1}$$

satisfying

$$B\mathbf{p} \leq \mathbf{b}, \tag{2}$$

where $B \in \mathbb{R}^{s\times k}$ and $\mathbf{b} \in \mathbb{R}^s$ are known. This restricts the solution space to a bounded convex polytope, C.

We present numerical experiments, which demonstrate that the stochasticity and uncertainty characterizing such a system can be captured by sampling parameter values which are distributed according to a prescribed probability density function f over C. Our first example explores the stochastic dynamics of a network of species, which mimics a food web model and where stochasticity in $\mathbf{p}$ is assumed to be an inherent attribute of the dynamics. Our second example involves uncertain parameters bounded by polyhedral uncertainty sets in an age-structured population dynamics model. The uncertainty sets are convex polyhedron with linear constraints that model fishing mortality in the statistical analysis of fisheries catch-at-age data. The examples illustrate a parsimonious approach to modeling complex systems under uncertainty.

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Boundary Conditions for Constrained Hyperbolic Systems: Mathematical and Numerical Analysis

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Many applications in sciences and technology lead to first order symmetric hyperbolic (FOSH) systems of differential equations supplemented by constraint equations. The Cauchy problem for many such FOSH systems is constraint-preserving, i.e., the solution satisfies certain spatial differential constraints whenever the initial data does (e.g., Maxwell's equations or Einstein's field equations in various FOSH formulations). Frequently, artificial space cut offs are performed for such evolution systems, usually out of the necessity for finite computational domains. However, it may easily happen that boundary conditions at the artificial boundary for such a system lead to an initial boundary value problem which, while well-posed, does *not* preserve the constraints. Therefore, boundary conditions have to be posed in such a way that the numerical solution of the cut off system approximates as best as possible the solution of the original problem on infinite space, and this includes the preservation of constraints. It has become increasingly clear that in order for constraints to be preserved during evolution, the boundary conditions have to be chosen in an appropriate way. Here we consider the problem of finding constraint-preserving boundary conditions for constrained FOSH systems in the well-posed class of maximal nonnegative boundary conditions. Based on a characterization of maximal nonnegative boundary conditions, we discuss a systematic technique for finding such boundary conditions that preserve the constraints, pending that the constraints satisfy a FOSH system themselves. We exemplify this technique by presenting a few relevant applications (e.g., for FOSH formulations of Einstein's equations and for systems of wave equations in FOSH formulation subject to divergence constraints).

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Nonconforming Generalized Finite Element Method for Linear Parabolic Interface Problems

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We propose a method for treating Dirichlet boundary conditions for linear parabolic interface problems in the framework of the Generalized Finite Element Method (GFEM). Let $\Omega \subset \mathbf{R}^n$ be a bounded domain with smooth boundary $\partial\Omega$. We consider the linear parabolic equation

$$u_t - \operatorname{div}(\mathscr{A}\nabla u) + a_0(x)u = f \quad \text{in } \Omega \times (0,T], \tag{1}$$

with initial and boundary conditions

$$u(x,0) = u_0 \quad \text{in } \Omega; \quad u(x,t) = 0 \quad \text{on } \partial\Omega \times (0,T], \tag{2}$$

and interface (or "jump") conditions

$$[u] = 0, \quad [\mathscr{A}\frac{\partial u}{\partial n}] = g(x,t) \quad \text{on } \Gamma, \tag{3}$$

where the *interface* Γ is a finite union of smooth, closed and disjoint surfaces, which do not intersect $\partial\Omega$, the boundary of Ω. The interface Γ together with $\partial\Omega$ partition Ω into k smooth subdomains Ω_l, $0 \le l \le k$, with Ω_0 the bordering subdomain. The forcing term f and initial data u_0 are assumed to be smooth in each subdomain Ω_l, $0 \le l \le k$. We assume that the coefficient matrix $\mathscr{A} = (a^l_{ij}(x))^n_{i,j=1}$, $0 \le l \le k$, is symmetric and piecewise smooth with the only possible jump discontinuities along Γ. We also assume that the coefficient matrix $\mathscr{A}$ is bounded and uniformly positive definite in each subdomain Ω_l, $1 \le l \le k$. The discontinuity of the coefficients arises from physical problems, e.g., for bodies that consist of two or more different materials. Solving such problems has important applications in non-stationary heat conduction problems, material sciences, fluid dynamics, etc.; see [4].

We consider a sequence of approximation spaces S_μ satisfying two conditions: (1) nearly zero boundary and interface matching, (2) approximability, which are similar to those my collaborators and I used in [1, 2, 3] for solving elliptic problems. Then, under certain regularity conditions for f, u_0 and g, if $u_\mu(t) \in S_\mu$, $\mu \ge 1$, is a sequence of continuous time Galerkin approximations of the solution u to the interface problem (1)-(3), the approximation error $\|u - u_\mu\|_{L^2(0,T;\hat{H}^1(\Omega)}$ is of order $O(h^m_\mu)$, where h^m_μ is the typical size of the elements in S_μ. Here $\hat{H}^1(\Omega)$ is the "broken" Sobolev space of functions in H^1 on each side of the interface. Optimal order error estimates can be obtained for the discrete time Galerkin method as well (e.g., by using the backward Euler scheme).

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Numerical Algorithm to Solve Two-Point Non-Linear Singularly Perturbed Boundary Value Problems Using Initial Value Technique

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In view of the wealth of literature on singular perturbation problems, we raise the question of whether there are other ways to attack singular perturbation problems, namely ways that are very easy to use and ready for computer implementation. It is easier to solve an initial value problem than solving its corresponding boundary value problem. So, many researchers in the field of numerical analysis have used the technique of reducing a given second order singularly perturbed boundary value problem to a system of first order equations which can then be solved using any known numerical method. In response to the need for a fresh approach to singular perturbation problems, the present paper builds an initial value technique for solving a two-point non-linear singularly perturbed boundary value problem. The original problem is reduced to an equivalent system of first order initial value problems which are then solved by the non-linear single step explicit scheme. Some numerical examples are given to illustrate the given method. It is observed that the presented method approximates the exact solution very well for crude mesh size h. Error analysis and convergence analysis of the method are also described.

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Simulation of a Tumor Growth Model Based on an Adaptive Markov Chain Monte Carlo (AMCMC) Method

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The complex and constantly involving nature of cancer has made it difficult to identify how the cellular and molecular components of cancer combine to influence clinical progression. Computer simulations based on mathematical models are important tools that can provide a robust framework to better understand cancer progression and response to therapies. With limited experimental data, the inference of mechanistic descriptions of oncogenesis becomes a challenge. AMCMC methods have been developed and widely used in Bayesian analysis. The objective of this study is to apply an AMCMC technique to calibrate the parameters of a tumor cell growth dynamics model to experimental data. In the AMCMC methods, the model is simulated repeatedly to explore the probability distribution describing the uncertainties in model parameters and predictions with successive steps weighed by the likelihood of experimental data given the parameter values. In the AMCMC method based on the Metropolis-Hastings algorithm, the proposal distribution needed by the algorithm learns from the target distribution as the simulation proceeds. The Gelman-Rubin potential scale reduction factor is applied to the model predictions to assess the convergence of the Markov Chains. The calibrated model captures the modest suppression of tumor cell growth in response to immunization in a mouse model for spontaneous melanoma. The calibrated model will provide a platform for in silico screening of the optimal therapeutic dosage and timing in mixed immuno-chemotherapies. The study has been supported by the National Institute of General Medical Sciences of the National Institutes of Health grant as part of the West Virginia IDeA Network of Biomedical Research Excellence (P20GM103434).

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Solving a Large Scale Thermal Radiation Problem Using an Interoperable Executive Library Framework on Petascale Supercomputers

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In this paper, we present a novel method to compute the transient thermal condition of a set of objects by solving the following conservative energy equations,

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot [k(x)\nabla T] - s(x,t) = 0 \tag{1}$$

$$k\nabla T \cdot n + h_{conv}(T - T_{atm}) + \sigma\varepsilon(T^4 - T_{ref}^4) + f(t) \cdot n = 0 \tag{2}$$

To compute the amount of heat transfer by conduction, convection, and radiation to and from the objects, the derived methodology exploits the heterogeneous architecture of the emergent supercomputers composed of CPUs and GPUs. While the energy equation (1) and the convective energy transfer, second term in equation (2), are formulated in finite element method and solved by the sparse iterative solvers derived from Trilinos [1], the amount of average radiating energy on a set of surfaces are prescribed by a linear system of the radiosity equations. The system of radiosity equations is simple to formulate but is challenging to solve when the number of Lambertian surfaces associated with an application becomes large. For an unsteady thermal problem in which the mesh configuration remains unchanged, the triangular factor of the symmetric radiosity matrix can be computed once and be reused subsequently in every time step. The radiosity matrix requires the computation of the view factors. Based on a serial view factor algorithm derived by Walton [2], we have extended his algorithm to compute the view factors on a parallel computer equipped with GPUs. A parallel Cholesky decomposition solver, based on a hybrid CPU/GPU ScaLAPACK library [3], is also built to factor and solve the matrix. The coupling and interplay of the direct radiosity solver using GPUs and the CPU-based FEM sparse solvers are handled by a light weight software integrator called Interoperable Executive Library (IEL) which manages the distribution of data and memory, coordinates communication among parallel processes, and directs execution of the set of loosely coupled physics tasks warranted by the thermal condition of the simulated object and its surrounding environment. A number of benchmarks are tested on keeneland, a GPU-based supercomputer at the National Institute for Computational Sciences(NICS). The methodology of the simulation will be presented in details. The benchmark results will be examined and presented.

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Discretization of Fractional Order Differentiator Over Paley-Wiener Space

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Functions that belong to the Paley-Wiener space *PW* are also known as bandlimited signals. The Paley-Wiener space is defined by $PW_B := \left\{ f : f \in L^2(\mathbb{R}^n) \cap C(\mathbb{R}^n),\ \operatorname{supp} \hat{f} \subseteq \bar{B} \right\}$, where $\hat{f}$ is the Fourier transform of f, i.e. the Fourier transform of the function is compactly supported in the Frequency domain. Analog fractional order differentiator can be represented by way of the Cauchy integral formula, special functions, as well as the Fourier/Laplace transformer, while digital differentiator of fractional order can be obtained through direct or indirect discretization techniques. In this work, we present the design of a finite impulse response (FIR) filter that discretizes the fractional differentiator over functions in Paley-Wiener space, which represent a large class of signals in digital signal processing. The proposed FIR model has the following characteristics: (a) the filter coefficients are independent of the signal samples; (b) it is capable of interpolating or extrapolating at an arbitrary point in the sampling domain; (c) it is adaptive to uniform or non-uniform sampling scenarios. We present explicit form of expressions on the matrices that lead to the computation of the filter coefficients. A closed form error bound is obtained to prove the accuracy of the proposed model along with numerical examples. The proposed filter is also used to generate fractal processes that are applicable for secure communications.

Numerical Methods for Differential-algebraic Equations and Applications (SS-NMDAEA)

Organizers:
Andreas Griewank (Humbold University)
Ned Nedialkov (McMaster University)
John Pryce (Cardiff University)

Many physical systems are naturally described by systems of differential-algebraic equations (DAEs). This minisymposium is devoted to recent developments in methods and software for DAEs. Topics include index determination, symbolic-numeric techniques, numerical integration schemes, and in particular schemes for high-index DAEs; schemes for structural analysis and integration using automatic differentiation. Methods for validated solution of ordinary differential equations by differential inequalities/inclusions are of interest, and especially extension of such methods to handle DAEs.

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Generalized Bessel Functions and Sturm Liouville Equations

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Atherosclerosis begins with the transport of low-density lipoprotein (LDL) across the monolayer of endothelial cells (ECs) that line and tile the vessel wall, and into the intima, where initial lipid accumulation takes place [2]. Some ECs have temporarily-widened junctions that allow passage of LDL. Laplace's equation describes the pressure distribution in the wall, whose gradient is proportional to the advecting velocity. This yields a boundary value problem with mixed Dirichlet/ Robin boundary conditions. The geometry of the problem is a rectangle that is divided into two smaller rectangles: media ω_1 and ω_2 with the two solutions $P_i(r,z)$,respectively for $i = 1,2$. We have previously solved the problem of the existence of the solutions $P_i(r,z)$ for the pressure of the blood flow [1]. For our present problem we considered solving an advectivediffusion equation (1) analytically whose solution $C_i(\tau,r,z)$ represents the solute concentration in the blood.

$$\frac{\partial C_i}{\partial \tau} + \nabla q_i = 0, \, i = 1,2 \tag{1}$$

In this equation $q_i(r,z)$ is a linear function of the derivative of the Pressure $P_i(r,z)$ i that we solved in our previous problem. The boundary conditions are again given in the above two regions with some of the boundary conditions are mixed Robin and Dirichlet conditions as in the previous problem. Thus, this is a more complicated Sturm- Liouville equation with coefficients given by a series of Bessel functions. To solve this problem we constructed a linear system of integral equations that approximate the coefficients of the series expansion of the solution. We proved the existence of the solution to this problem analytically by using Gershgorin's theorem on the location of the eigenvalues of the corresponding matrix.

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Symbolic Application of the Pryce Σ–Method for Index-Reduction of DAEs in CyModelica

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The Pryce Σ-Method [1] is a technique for structural-analysis of Differential Algebraic Equations (DAEs) applicable to general sets of DAEs containing derivatives of any order. The output of an analysis is the number of times to differentiate each equation. Previous applications of this technique [2, 3] have focused on the construction of Taylor series for the numerical solution of the problem using automatic differentiation.

This contribution describes an alternative approach to those previously described of using the Σ-Method for the solution of a set DAEs of unknown index. The results of the structural-analysis are applied symbolically to the system of equations, utilizing the information to apply a variation of the dummy-derivatives [4] method. This involves selectively differentiating equations and appending them to the problem to be solved, while also disassociating selected states from their derivatives in order to maintain an equal number of unknowns to equations and to avoid drift due to the numerical integrator.

Potential pitfalls at this stage will be discussed and how further symbolic analysis of the differentiated equations is performed and applied in order to mitigate these.

These techniques are applied in CyModelica [5], a commercial compiler and simulator for the Modelica [6, 7] open-standard modeling language. Modelica enables the construction of equation-based models of complex systems for simulation. These can include a mixture of domains, such as mechanical, electrical and thermodynamic systems, and the interactions between them. This paper describes how the symbolic techniques introduced are applied to such a problem in order to utilize general numerical techniques to perform efficient simulation.

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Structural analysis and dummy derivatives - some relations.

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Differential algebraic equations, DAEs, appear frequently in applications involving equation based modelling, from robotics to chemical engineering. A common way of making a DAE amenable to numerical solution is by reducing the index to get a corresponding ODE and using an ODE solution method. The signature matrix method developed by Pryce does not rely on an index reduction step and instead solves the DAE directly via Taylor series [1]. The talk will draw comparisons between these two different approaches and show the signature matrix method is in some sense equivalent to the dummy derivative index reduction method developed by Mattsson and Söderlind [2]. The talk will draw on standard examples from the DAE literature, such as the simple pendulum and the Campbell-Griepentrog robot arm [3], to illustrate the connection between the two methods.

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A Simple Method for Quasilinearity Analysis of DAEs

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We consider systems of DAEs of any order. If the leading derivatives in a DAE appear in a jointly linear way, we say it is quasilinear. We present a simple method for extracting quasilinearity information from the function defining the DAE. In our method, we use the offsets obtained from Pryce's structural analysis [1] and determine for each equation if it is quasilinear in its leading derivatives. This can be done through operator overloading or source code translation.

Using this information, and a block-triangularization of the DAE [2], we can often reduce the number of required initial conditions. Furthermore, systems that are non-quasilinear may break down into smaller, quasilinear systems, which can be solved more efficiently compared to solving the whole system. Our method has been implemented using operator overloading in the DAETS solver [4] and in the DAESA [3] structural analysis tool.

We outline the underlying algorithms, illustrate them on several examples, and elaborate on implementation issues.

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Progress on the DAESA tool for structural analysis of DAEs

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Large DAE systems are produced by equation-based modeling methods in many engineering and scientific disciplines. It is now routine that they are generated by software using interactive systems such as gPROMS or DYMOLA. Mostly these have some kind of structural analysis (SA) of the DAE built in.

For some years the authors have been developing a numerical code DAETS for solving DAEs. It is based on a SA of the sparsity of the DAE that we call the signature matrix method. In many ways it is equivalent to the well-known method of Pantelides, and computes the same structural index, but it is easier to use.

Originally, our SA was merely a preprocessing stage to set up the numerical solution method for DAETS. However, as we have encountered users with increasingly large problems, it has become clear that they value its diagnostic abilities, not all of which are present in other systems, although there is a large overlap. In particular, our SA is able to identify subsystems of a DAE to a finer resolution than many other methods. Thereby, it can often reduce the number of initial values required for numerical solution, beyond what those other methods achieve—a useful feature in view of the notable difficulty of estimating consistent initial values for a DAE.

Thus it seemed useful to present it as a free-standing tool, with enhanced reporting and diagnostic capabilities. The result is the program DAESA. Written in MATLAB, it accepts a MATLAB description of a DAE similar to the C++ description accepted by DAETS.

DAESA is under active development. The talk will show examples of its use on small and on larger problems. We would welcome discussion of how its SA compares with that of other systems and how to improve it further.

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Optimization of large-scale DAE systems in chemical process design and control using parallel computing

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Modeling and optimization using differential-algebraic equations (DAEs) is ubiquitous in chemical process design and control. A particularly interesting application is the integration of design and control via dynamic optimization-based strategies, which offer a systematic approach to combat poor control performance, violation of safety and environmental constraints, and degradation in economic performance. In order to construct a realistic design problem, uncertainty must be explicitly embedded within the DAE system that describes possible unknown exogenous disturbances and model parameters. One approach to incorporating uncertainty into such formulations is using a so-called multi-period (or multi-scenario) discretization of the infinite dimensional uncertainty space ($\Gamma = \{\boldsymbol{\theta} | \boldsymbol{\theta}^L \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^U\}$), which results in numerous discrete realizations ($\boldsymbol{\theta}^{(i)}$ for $i = 1, \ldots, n_s$) [1]. General multi-period dynamic nonlinear programs (using an embedded first order DAE – written in implicit form via $\mathbf{F}(\cdot)$) can be stated as follows:

$$
\begin{aligned}
\min_{\mathbf{d}} \; & \mathcal{J} := f_d(\mathbf{d}) + \textstyle\sum_{i \in \mathcal{S}} w_i \cdot \phi_i(\mathbf{x}^{(i)}(t), \mathbf{z}^{(i)}(t), \mathbf{v}^{(i)}(t), \mathbf{d}, \boldsymbol{\theta}^{(i)}) \\
\text{st:} \; & \mathbf{F}_i(\dot{\mathbf{x}}^{(i)}(t), \mathbf{x}^{(i)}(t), \mathbf{z}^{(i)}(t), \mathbf{v}^{(i)}(t), \mathbf{d}, \boldsymbol{\theta}^{(i)}) = \mathbf{0}\,, \quad \mathbf{x}^{(i)}(t_0) = \mathbf{h}_{0,i}(\mathbf{d}, \boldsymbol{\theta}^{(i)}) \\
& \mathbf{h}_i(\dot{\mathbf{x}}^{(i)}(t), \mathbf{x}^{(i)}(t), \mathbf{z}^{(i)}(t), \mathbf{v}^{(i)}(t), \mathbf{d}, \boldsymbol{\theta}^{(i)}) = \mathbf{0} \\
& \mathbf{g}_i(\dot{\mathbf{x}}^{(i)}(t), \mathbf{x}^{(i)}(t), \mathbf{z}^{(i)}(t), \mathbf{v}^{(i)}(t), \mathbf{d}, \boldsymbol{\theta}^{(i)}) \leq \mathbf{0} \\
& \mathbf{d} \in [\mathbf{d}^L, \mathbf{d}^U] \quad \forall\, i \in \mathcal{S} = \{1, \ldots, n_s\}
\end{aligned}
\tag{P1}
$$

where $\mathbf{x}(t)$, $\mathbf{z}(t)$ represent differential and algebraic states, respectively; $\mathbf{v}(t)$ are prescribed disturbances; $\mathbf{d}$ are system design parameters. Such discretizations yield large and potentially unwieldy systems of DAEs, which must be solved in an efficient manner. Fortunately, the resulting uncertainty discretization and the fundamental multiple-shooting dynamic optimization approach that we have adopted [2], allows for the DAE solution to be implemented in a highly parallel manner.

Our focus of this talk will be on describing an algorithm for efficiently solving such large-scale multi-period DAE representations and its use within integrated design and control applications for improving computational performance. A unique aspect of our investigation is the combination of a multiple-shooting solution approach within a multi-period formulation, where our objective is increasing NLP solution speed through parallelizing the DAE integration tasks over each shooting interval and scenario realization. Realistic industrial case studies will be presented and numerical results (parallel speedup and efficiency) investigated and discussed; additionally, avenues for future research will be identified.

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Quantum Control: Theory and Application (SS-QCTA)

Organizer:
Lian-Ao Wu (IKERBASQUE, Basque Foundation of Science, University of the Basque Country)

Control of quantum dynamics is of great interest and has become a general theme at the frontier of science and technology, driven by the latest technological developments in femtosecond laser physics, state-selective physical chemistry, materials synthesis, quantum information processing and quantum computing. While quantum control theory has been formulated based on fundamental quantum mechanics, its theoretical applications in specific areas, such as control of open systems, are still in progress. This session will focus on the recent developments of quantum control theory and its applications. In particular, master equation approaches of open systems, dynamical control, quantum simulations using optical lattices, spin ensembles, ultra-cold atoms, etc.

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Experimental Novel and Robust Quantum Control of Single Electron Spin in Diamond

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An accurate control over the dynamics of open systems is of great importance for nowadays quantum physics and engineering, such as quantum information processing, high resolution spectroscopy and quantum metrology. First, we report an experiment which demonstrates a robust control of an electron spin via continuous-wave dynamical decoupling (CWDD) method. The result shows that CWDD shares the merits of retaining the superiority of prolonging the coherence time and at the same time easily combining with quantum logic tasks. Second, we experimentally demonstrated universal quantum control of a single electron spin in diamond via SUPCODE, a type of dynamically corrected gates (DCGs). The decoherence effect, which is introduced by the nuclear spin bath, has been suppressed up to sixth order with five-piece SUPCODE pulses. Third, a novel manner of quantum manipulation is experiment demonstrated by using a nitrogen-vacancy (NV) center spin in diamond. We observe for the first time Rabi oscillations of the electron spin resulting from the interference between successive Landau-Zener processes in various regimes, including both slow and fast passage.

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Scaling of Spin Qubit Decoherence in Semiconductors

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A crucial issue in spin-based quantum information processing is spin coherence. Decoherence of a single electron spin confined in a quantum dot or to a donor ion has been studied extensively, with hyperfine interaction to the environmental nuclear spins being identified as the most important channel of spin decoherence [1]. Decoherence of multiple-spin-qubit states is inevitably affected by singe-spin decoherence. Moreover, for exchange-coupled spin qubits, there are new decoherence channels beyond those for single spins because of the Coulombic nature of the exchange interaction [2]. Here we discuss our studies of two-spin [3] and three-spin [4] decoherence, including both known single-spin decoherence channels due to nuclear spins and new channels based on electrostatic coupling. Our results show that nuclear spins affect two- and three-spin states in a qualitatively similar manner as for single spin states, although there are interesting new twists when the orbital symmetry may lead to weaker hyperfine interaction. On the other hand, phonon induced dephasings depend strongly on the electrical features of the nanostructure, and could pose another constraint on two-qubit gates and quantum computing schemes based on two- and three-spin encoding [5].

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Correlation Dynamics and Scaling Behavior of Two-Qubit System in the Spin-Chain Environments

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We study the dynamics of classical and quantum correlations for a two-qubit system in an XY spin-chain environment. A sudden transition is found to exist between classical and quantum decoherence with certain initial states. We show that the sudden transition happens near the critical point and it provides an alternative way to characterize the quantum phase transition. The environmental parameters have strong influence on the quantum discord (QD) decay rates. An interesting scaling behavior for the QD is obtained in the weak coupling limit. In the strong coupling limit, the classical correlation (CC) and the QD oscillate with time rapidly, but present regular distributions under a specific time interval. In addition, the decay parts of the CC and QD envelopes show Gaussian feature.

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Tight-binding models for ultracold atoms in honeycomb optical lattices

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We discuss how to construct tight-binding models for ultracold atoms in honeycomb potentials, by means of the maximally localized Wannier functions (MLWFs) for composite bands introduced by Marzari and Vanderbilt [Phys. Rev. B **56**, 12847 (1997)]. In particular, we work out the model with up to third-nearest neighbors, and provide explicit calculations of the MLWFs and of the tunneling coefficients for the graphene-like potential with two degenerate minima per unit cell. Finally, we discuss the degree of accuracy in reproducing the exact Bloch spectrum of different tight-binding approximations, in a range of typical experimental parameters.

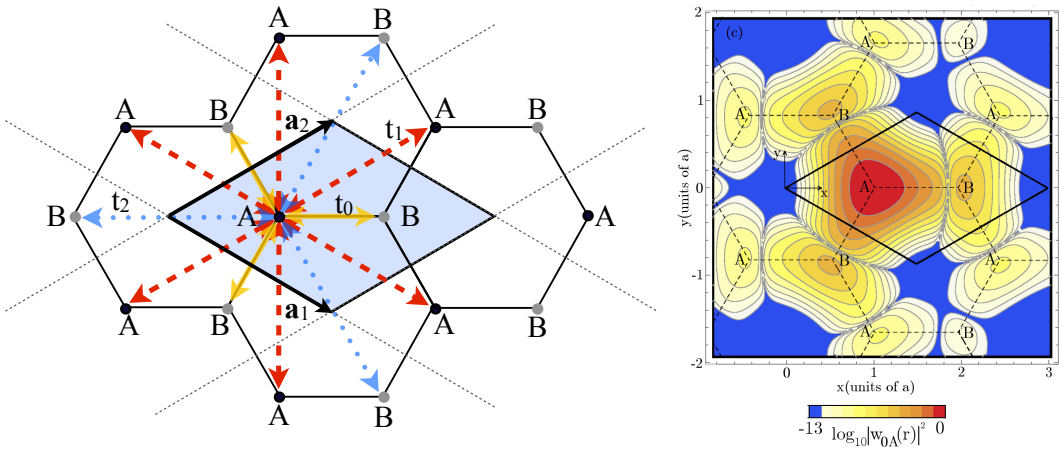

Figure 1: (left) Sketch of the honeycomb lattice structure and the diamond-shaped elementary cell with basis *A* and *B*. The different types of tunneling considered are indicated for a site of type A. (right) Example of the calculated MLWFs. The solid and dashed lines depict the original unit cell and honeycomb lattice, respectively.

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Fast and Robust Spin Manipulation in a Quantum Dot by Electric Fields

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Spin-orbit coupling allows for a direct spin manipulation by external time-dependent electric field [1,2]. However, the optimal strategy for this procedure has yet to be designed. Usually a periodic electric field is assumed to be applied to flip electron spin in a quantum dot [1]. However, corresponding Rabi frequency is rather low making the entire process prone to decohence. Here we propose a different approach and apply an invariant-based inverse engineering method to control, by time-dependent electric fields, the spin dynamics in a quantum dot in a weak magnetic field in the presence of a spin-orbit coupling of the Rashba and Dresselhaus types. The designed electric fields provide a shortcut to adiabatic processes that flip the spin rapidly, thus avoiding decoherence effects. This approach, being robust with respect to the device-dependent noise, can open new possibilities for spin-based quantum information processing.

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Remarks on the (non-)controllability of Schrödinger equations

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After briefly reviewing some known results (focusing on exact control), I will discuss some of the obstacles to controllability and techniques for showing non-controllability specific to Schrödinger equations.

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Cooling and Probing a Nanomechanical Resonator Coupled to a Double Quantum Dot

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We study the cooling of a nanomechanical resonator (NAMR) that is capacitively coupled to a double quantum dot (DQD). The NAMR is cooled by the dynamical backaction induced by the capacitive coupling between the DQD and the NAMR. The DQD is excited by a microwave field and afterwards a tunneling event results in the decay of the excited state of the DQD. An important advantage of this system is that both the energy level splitting and the decay rate of the DQD can be well tuned by varying the gate voltage. We find that the steady average occupancy, below unity, of the NAMR can be achieved by changing both the decay rate of the excited state and the detuning between the transition frequency of the DQD and the microwave frequency, in analogy to the laser sideband cooling of an atom or trapped ion in atomic physics. Our results show that the cooling of the NAMR to the ground state is experimentally implementable.

Moreover, we propose a current correlation spectrum approach to probe the quantum behaviors of the NAMR coupled to a DQD. This DQD acts as a quantum transducer and is further coupled to a quantum-point contact (QPC). By measuring the current correlation spectrum of the QPC, shifts in the DQD energy levels, which depend on the phonon occupation in the NAMR, are determined, and thus quantum behaviors of the NAMR could be observed. In particular, the cooling of the NAMR into the quantum regime could be examined. In addition, the effects of the coupling strength between the DQD and the NAMR on these energy shifts are studied. We also investigate the impacts on the current correlation spectrum of the QPC due to the backaction from the charge detector on the DQD.

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Recent Progress in Spintronics: Experiment, Theory and Simulation (SS-RPSETS)

Organizers:
Jingrun Chen (University of California Santa Barbara)
Xu Yang (University of California Santa Barbara)

Spintronics refers to the active control and manipulation of spin degrees of freedom in solid-state physics. Its study is challenging, as it involves a number of processes at different time and length scales: polarization of the spin, transport and diffusion of the polarized spin between the ferromagnetic layers, and interaction with the underlying magnetization. Experimental results show that exploiting the spin of the electron can lead to technological advances and the design of devices with new functionality. The objective of this minisymposium is to bring together specialists in the field from different backgrounds, and facilitate the exchange of ideas and recent developments. Topics on experiment, theory and simulation will be discussed.

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An Introduction to Spin Effects in Organic Solar Cells

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In organic solar cells, the exciton-phonon interaction is considered as the mechanism for spin flipping which can change an exciton from the singlet state to the triplet state. Subsequently, some properties in the organic material will be changed. For example, very large exciton diffusion length was observed for triplet excitons. In this talk, spin effects in organic solar cells will be reviewed.

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Spin-polarized currents in ferromagnetic multilayers

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We present a semi-implicit numerical method for micromagnetics simulations, in the presence of spin-currents. The dynamics of the magnetization are described by the Landau-Lifshitz-Gilbert equation, while the dynamics of the spin are described by a diffusion equation with discontinuous coefficients. The complexity of the method presented is comparable to that of solving the linear heat equation with the Backward Euler method. To illustrate the procedure, we carry out three dimensional simulations of the magnetization reversal process in a magnetic multilayer when a current flows perpendicular to the layers. Spin-polarized currents are shown to decrease the coercive field, and to induce magnetization reversal even in the absence of external magnetic fields.

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Magnetic Ordering and Thermally Enhanced Magnetism in Quantum Dots

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Magnetic quantum dots (QDs) can be viewed as tunable nanomagnets providing an enhanced control of magnetic ordering as compared to their bulk-like counterparts [1, 2]. Recent experimental advances in fabricating such structures, both as epitaxially grown self-assembled QDs [3] and solution processed colloidal nanocrystals [4, 5], pose interesting challenges for their modeling. On one hand, a widely used mean-field description of magnetism ignores fluctuations in magnetization. Fluctuation effects are essential for these nanomagnets, as these systems are too small to be in a thermodynamic limit. A prime example, is the formation of a magnetic polaron (MP). A MP can be viewed as a cloud of localized impurity spins, aligned through exchange interaction with a single localized carrier (electron or hole) spin. A mean-field solution gives spurious phase transitions which are removed when fluctuations are taken into account. On the other hand, high photo-excitation experiments can create multiple carrier occupancies in the QDs. Therefore, we need to generalize the concept of MP. We show that double occupancy (two electron or holes) can lead to the formation of a magnetic bipolaron (MBP) [6, 7] and several surprising effects e.g. (i) magnetic ordering is even possible in a closed shell system (expected, like noble gases, to be magnetically inert), (ii) thermally enhanced magnetic ordering [8], (iii) nonmonotonic behavior of experimentally observable photoluminescence. We show that the standard mean-field treatment of MPs and MBPs leads to unphysical phase transitions. We reveal how this spurious effect is removed when fluctuations are correctly taken into account. Our studies of magnetic ordering, motivated also by recent experiments [3] in (Zn,Mn)Te/ZnSe QDs, are corroborated by independent Monte Carlo simulations [9]. This work was supported by DOE-BES, AFOSR-DCT, U.S. ONR, and NSF-DMR.

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Domain Wall Trajectory Determined by its Fractional Topological Edge Defects

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The theory of topological defects has had a significant influence on the understanding of various physical phenomena ranging from superfluid Helium-3 to liquid crystals. Topological defects are general features in systems with broken symmetries such as head-to-head (HH) and tail-to-tail (TT) domain walls (DWs) in soft ferromagnetic nanowires (NWs). Such DWs are further composed of elementary topological bulk and edge defects with integer and fractional winding numbers, respectively; whose relative spatial arrangement determines the chirality of the DW. Understanding the influence of the DW structure on its motion is critical for both fundamental and technological reasons. In this talk, we will show how one can understand and control the trajectory of DWs in magnetic branched networks, composed of connected NWs, by a consideration of their fractional elementary topological defects and how they interact with those innate to the network. We will describe a simple yet a highly reliable mechanism that we have developed for the injection of a DW of a given chirality into a NW and exploit it to show that it is the DW's chirality that determines which branch the DW follows at a symmetric Y-shaped magnetic junction - the fundamental building block of the network. Using these concepts, we will unravel the microscopic origin of the one-dimensional (1D) nature of magnetization reversal of artificial spin ice systems that have been observed in the form of Dirac strings. This understanding will allow for the formation of more complex chiral magnetic orders by controllably generating and propagating several domain walls of specific chiralities into artifical spin ice structures to form defined lattices of Dirac strings.

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Switching current and thermal stability of perpendicular-anisotropy CoFeB-MgO based magnetic tunnel junctions

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Nonvolatile logic and memory are attracting much attention because those have a potential in offering reductions of power consumption and interconncetion delay [1]. Magnetic tunnel junction (MTJ) is a candidate for their building block, and therefore intensively studied. It was reported that CoFeB-MgO MTJ with perpendicular easy-axis (p-MTJ), where perpendicular magnetic anisotropy is attributed to intrefacial anisotropy at CoFeB-MgO interface [2], have a high potential to be used with CMOS logic [3]; high tunnel magnetoresistance (> 100%), low intrinsic critical current (I_{C0} ~ 50 μA), a relatively high thermal stability factor (Δ ~ 40), and annealing stability up to 350°C at a junction size of 40 nm in diameter. Δ of CoFeB-MgO shows almost constant value down to critical size [4, 5], below which Δ starts to decrease [6]. We showed that Δ of CoFeB-MgO p-MTJs increase linearly with increasing the recording layer thickness [7]. Since perpendicular magnetic anisotropy of CoFeB-MgO system is originated from interfacial anisotropy, use of double CoFeB-MgO interfaces allow one to increase the recording layer thickness while keeping perpendicular easy axis. We adopted MgO/CoFeB/Ta/CoFeB/MgO recording layer structure to increase the recoding layer thickness in which Ta thin layer was inserted for boron absorption from CoFeB layers [8]. Results show that Δ increases by a factor of 1.9 in the recording structure with comparison to that of single-interface CoFeB-MgO p-MTJs at a junction size of 70 nmϕ while keeping comparable I_{C0}. In similar p-MTJs with double-interface, higher Δ compared to those with single-interface was also reported [9, 10]. We further studied the recording structure at a reduced dimension of 29 nmϕ where high Δ of 59 was obtained [11].

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Effective dynamics of electrons in crystal

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We study the dynamics of interacting electrons based on the time dependent density functional theory. Specifically we derived the homogenized Maxwell equations for crystalline insulator. The dynamics of electrons were considered in the high frequency regime under the external macroscopic electromagnetic fields.

Recent Trends in Differential Equations and Dynamical Systems (SS-RTDEDS)

Organizers:
Xinzhi Liu (University of Waterloo)
Mohamad Alwan (University of Waterloo)
Hongtao Zhang (University of Waterloo)

There has been much progress in differential equations and dynamical systems in recent years. This session will consist of several leading experts and active researchers to give lectures that cover the recent trends in this area.

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Input-to-State Stability of Large-Scale Stochastic Impulsive Systems with Time Delay and Application

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This paper deals with large-scale nonlinear delay stochastic systems where the system states are subject to impulsive effects and perturbed by some input uncertainty having bounded energy. The random noise is represented by a Wiener (or Brownian motion) process, and the time delay is finite. Precisely, the interest is to establish the property of input-to-state stability in the mean square. A Vector Lyapunov function, Razumikhin-type technique, and comparison principle are used to develop Lyapunov-like sufficient conditions to prove the qualitative properties. Some special cases and application to a control system are given to justify the theoretical results.

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Viability for a time-dependent domain with respect to a reaction-diffusion system with delay

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Let X, Y be real Banach spaces, let $I=[a,b)\subseteq \mathrm{R}$ be a nonempty and bounded interval and let $A: D(A)\subseteq X\to X$ and $B: D(B)\subseteq Y\to Y$ be the infinitesimal generators of two C_0-semigroups.

If Z is a Banach space and $\sigma>0$, we denote by $C_\sigma^Z=C([-\sigma,0];Z)$ endowed with the norm

$$\|\psi\|_{\sigma;Z}=\sup\{\|\psi(t)\|_Z;\ t\in[-\sigma,0]\}.$$

If $w\in C([\tau-\sigma,T];Z)$, where $Z=X$ or $Z=Y$, then for each $t\in[\tau,T]$ we denote by $w_t\in C_\sigma^Z$ the function

$$w_t(s)=w(t+s) \text{ for } s\in[-\sigma,0].$$

Let $K: I\rightsquigarrow X\times Y$ be a multi-function with nonempty values, let

$$\mathcal{K}=\{(t,\psi,\eta)\in I\times C_\sigma^X\times C_\sigma^Y;\ (\psi(0),\eta(0))\in K(t)\}.$$

and let $F:\mathcal{K}\rightsquigarrow X$ and $G:\mathcal{K}\rightsquigarrow Y$ be two multi-functions with nonempty, convex and weakly compact values. Our aim here is to prove some new necessary and sufficient conditions in order that $\mathcal{K}$ be viable with respect to the delay reaction-diffusion system

$$\begin{cases} u'(t)=Au(t)+f(t), & f(t)\in F(t,u_t,v_t),\ \ t\geq\tau,\\ v'(t)=Bv(t)+g(t), & g(t)\in G(t,u_t,v_t),\ \ t\geq\tau, \end{cases} \tag{1}$$

which means that for each $(\tau,\psi,\eta)\in\mathcal{K}$, there exist $T>\tau$ and a continuous function $(u,v):[\tau-\sigma,T]\to X\times Y$ satisfying $(t,u_t,v_t)\in\mathcal{K}$ for $t\in[\tau,T]$ and (u,v) is a mild solution of the system (1) satisfying $u(t)=\psi(t-\tau)$ and $v(t)=\eta(t-\tau)$ for $t\in[\tau-\sigma,\tau]$. Of course, it is understood that $f\in L^1(\tau,T;X)$ and $g\in L^1(\tau,T;Y)$.

For previous viability results on abstract reaction-diffusion systems without delay see: Burlică [1], Burlică and Roşu [2], Necula and Vrabie [4], Roşu [5] and the references therein.

We emphasize that our main theorem is a nontrivial extension to abstract reaction-diffusion systems of a very recent result of Necula and Popescu [3].

In order to illustrate to power of our abstract result, we prove the existence of monotone solutions to a specific reaction diffusion system, i.e. for $X=Y=L^1(\Omega)$ with Ω a bounded domain in $\mathbb{R}^n$ with sufficiently smooth boundary Γ, $A=\alpha\Delta$ and $B=\beta\Delta$ subjected to Dirichlet boundary conditions, where $\alpha>0$ and $\beta>0$.

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Classification of Solutions of Second Order Nonlinear Neutral Delay Dynamic Equations

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In this paper, the oscillatory and nonoscillatory behaviour of solutions of the nonlinear neutral dynamic equations

$$[r(t)[x(t)+c(t)x(\alpha(t))]^{\Delta}]^{\Delta}+p(t)f^{\sigma}(x(\beta(t)))-q(t)g^{\sigma}(x(\gamma(t)))=0, \quad t\geq t_0 \tag{1}$$

are discussed. Where $c,r,p,q\in C_{rd}([t_0,\infty)_{\mathbb{T}},\mathbb{R})$ with $q(t),r(t)>0; f,g\in C_{rd}(\mathbb{R},\mathbb{R}); \alpha,\beta,\gamma\in C_{rd}(\mathbb{T},\mathbb{T})$, and $\alpha(t),\beta(t),\gamma(t)\leq t$ increasing and $\lim_{t\to\infty}\alpha(t)=\lim_{t\to\infty}\beta(t)=\lim_{t\to\infty}\gamma(t)=\infty$, and $\sigma:\mathbb{T}\to\mathbb{T}$ is a forward operator given by $\sigma(t)=\inf\{s\in\mathbb{T}:s>t\}$ for all $t\in\mathbb{T}$. We consider two cases, $p\geq 0$, and p changes sign, and give sufficient conditions for every solutions of equation (1) oscillate and also investigate asymptotic behaviour of nonoscillatory solutions. Examples are given to validate our results.

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A class of reaction-diffusion systems with mixed initial conditions

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We prove a global existence, uniqueness and uniform asymptotic stability result for C^0-solutions to a class of nonlinear delay reaction-diffusion system subjected to mixed initial conditions

$$(1)\qquad \begin{cases} u'(t) \in Au(t) + F(t, u_t, v_t), & t \in \mathbb{R}_+, \\ v'(t) \in Bv(t) + G(t, u_t, v_t), & t \in \mathbb{R}_+, \\ u(t) = p(u)(t), & t \in [-\tau, 0], \\ v(t) = \varphi(t), & t \in [-\tau, 0]. \end{cases}$$

Here X, Y are Banach spaces, $A : D(A) \subseteq X \rightsquigarrow X$, $B : D(B) \subseteq Y \rightsquigarrow Y$ are m-dissipative operators, $\tau \geq 0$, while $F : \mathbb{R}_+ \times C([-\tau, 0]; \overline{D(A)}) \times C([-\tau, 0]; \overline{D(B)}) \to X$ and $G : \mathbb{R}_+ \times C([-\tau, 0]; \overline{D(A)}) \times C([-\tau, 0]; \overline{D(B)}) \to Y$ are jointly continuous and Lipschitz with respect to their two last arguments and $p : C_b([-\tau, +\infty); \overline{D(A)}) \to C([-\tau, 0]; \overline{D(A)})$ is nonexpansive and the initial history $\varphi \in C_b([-\tau, +\infty); Y)$.

If $Z \subseteq X$, $C_b(I; Z)$ denotes the space of all bounded and continuous functions from the interval I to X, satisfying $u(t) \in Z$ for each $t \in I$ equipped with uniform convergence topology. As usual, if $u \in C_b([-\tau, +\infty); X)$ and $t \in [0, +\infty)$, $u_t : [-\tau, 0] \to X$ denotes the continuous delayed function defined by $u_t(s) := u(t+s)$ for each $s \in [-\tau, 0]$. Similarly, one defines $C_b(I; Y)$, $C_b(I; \overline{D(B)})$ and v_t.

We notice that, $p(u)(t) = u(t + 2\pi)$ for $t \in [-\tau, 0]$, leads to a 2π-periodic condition for the unknown function u, while $p(u)(t) = -u(t + 2\pi)$ for $t \in [-\tau, 0]$, yields a 2π-anti-periodic condition. Further, if the function p is defined by $p(u)(t) = \int_\tau^{+\infty} k(t, s)u(t + s)ds$, we obtain a mean condition on u.

For previous results on abstract reaction-diffusion systems subjected to initial or to periodic conditions see: Burlică [1], Burlică and Roşu [2], Díaz and Vrabie [5], Necula and Vrabie [7], Roşu [8] and the references therein.

The increasing interest in the study of such kind of evolution equations and systems with nonlocal initial conditions is motivated by the fact that they represent mathematical models of various phenomena, as for instance those described in Deng [4] and McKibben [6, Section 10.2, pp. 394–398]. The results in this talk will appear in Burlică, Roşu and Vrabie [3].

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Orthogonal separation of variables in spaces of constant curvature

Roman Smirnov

We will review some recent advances in the theory of orthogonal separation of variables within the framework of the invariant theory of Killing tensors.

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Power geometry for a reversible system of ordinary differential equations

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We consider reversible system of ODEs fourth order depending on two small parameters $X'' = (x_5, x_6)$:

$$\dot{X}' = \Phi(X', X''), \quad X' \in R^4, \quad \dot{X}'' = 0, \quad X'' \in R^2. \tag{1}$$

Here $X = (X', X'')$, $X' = (x_1, x_2, x_3, x_4)$, where $\Phi(0, X") = 0$, and the point $X' = 0$ is stationary, and the matrix of the unperturbed linear part L in $X = 0$ is a Jordan block with four-fold zero eigenvalue. Also it is supposed, system (1) is invariant under the substitution $X', X'', t \to SX', X'', -t$, where $SX' = (x_1, -x_2, x_3, -x_4)$, i.e. the property of reversibility of system (1) means that

$$S\Phi(X', X'') = -\Phi(SX', X''). \tag{2}$$

Such a system appears in Hydrodynamics. For example, the problem of surface water waves for the Bond number b close to $1/3$ and the Froude number $\widetilde{\lambda}$ close to 1 is transformed into system (1) as a result of reduction on the center manifold (see [3]).

The solutions to the system (1) are studied in the neighborhood of the stationary point $X = 0$ in the following way. The linear part of system (1), which depends on parameters, is reduced to the normal form. The lower triangular matrix of parameters is obtained, in such a way that each its diagonal consists of equal parameters. In the second diagonal from below and in the main diagonal there are only zeros because of the property (2). We discover the support $D \in R^6$ of system (1), i.e. the set of power exponents and using it we computed Newton polyhedron in R^6 by the program (see [1-2]). With the table of correspondence we extract all the set of truncated systems. We obtained only five truncated systems of maximal "dimension" five. Among them there is the basic truncated system which after the power transformation (see [1-2]) which the number of parameters is reduced to one and this system is reduced to the system

$$\dot{y}_1 = y_2, \quad \dot{y}_2 = \sigma y_1 + y_3, \quad \dot{y}_3 = \sigma y_2 + y_4, \quad \dot{y}_4 = \nu y_1 + \sigma y_3 + a y_1^2, \tag{3}$$

where $\sigma = \pm 1$,parameters ν and $a \in R$. It is shown that system (3) is a Hamiltonian one and it has only two independent quadratic first integrals. The main result of this work is the existence of new families of periodic waves and of new families of quasi-periodic waves for $\nu < 0$, which we have received.

Here we demonstrated the effectiveness of methods of Power Geometry (see [1,4]) for the investigation of rather complicated singularities on the example of system (1). We tried to use as simple algorithms of computations as possible, which allowed us to complete computations to the end.

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Recent results on stability of open-loop and closed-loop switched systems

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There has recently been an increased interest in the study of switched systems, which are systems that evolve according to mode-dependent dynamics and experience abrupt changes between modes, triggered by threshold events. These types of systems can model interesting and important problems in many different fields of research, such as applied mathematics, control engineering, computer science, and biology. From a control perspective, it may be possible to stabilize a system using switching control, where continuous control is not suitable or cannot be found. In this talk, two stabilizing switching control strategies are analyzed and compared: the first is time-dependent switching control (the open-loop switched control problem), where the switching rule and switching times are programmed into the data in advance. The second approach is using state-dependent switching control (the closed-loop switched control problem), where a state-dependent switching rule is constructed that uses the current state of the system. Switched systems with nonlinearities, delays, and impulses are considered and sufficient conditions are given which guarantee stabilization.

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An Explicit Recursive Formula for Computing the Normal Form and Center Manifold of n-dimensional Differential Systems Associated with Semisimple Cases

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Normal form theory is usually applied in the study of nonlinear differential systems together with center manifold theory. Using center manifold theory could help us find a locally invariant manifold with smaller dimension. Normal form theory is to introduce a series of nonlinear transformations to the center manifold and to get a new simpler system without topological structure being changed around a singular point. Hence a new system in a simpler form could be derived when both these theories are applied.

There are two critical parts in the computation of normal forms, computer algebra systems and methodologies. A computer algebra system, like Maple or Mathematica, must be used in computing normal forms, particularly when higher-order normal forms are needed. Several computationally efficient methodologies have been developed in the past decade, such as the method of multiple time scales combined with a perturbation technique and the method of Poincaré-Lyapunov constants, see Refs. [1, 2, 3]. These methods have been applied to a number of singularities such as Hopf, Hopf-zero, double Hopf, etc.

In this talk, we focus on general n-dimensional systems associated with semisimple cases, i.e. the Jacobian matrix of the linearized system evaluated at a singular point can be transformed into a diagonal Jordan canonical form. For the normal form and center manifold, an explicit, computationally efficient, recursive formula is presented, based on the coefficients of the original differential systems. Maple program is also developed based on the analytical formulas, and shown to be computationally efficient, with illustrative examples.

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Chaos Entanglement: Leading Unstable Linear Systems to Chaos

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Chaos phenomena, characterized by the so-called “butterfly effect" [1], are found in many fields such as physics, biology, philosophy, economics, engineering, etc. Due to its sensitivity to initial conditions and unpredictable essence, chaos has attracted significant attention since Lorenz published his landmark study on a mathematical model for weather prediction in 1963 [2]. The interest in chaos phenomenon is shifting the focus from eliminating chaos at the early stage to applying chaos in practice recently. Specifically, since chaos synchronization was presented by Pecora and Carroll in 1990 [3], chaotic systems became useful tools in engineering applications, for instance, the chaotic carrier for secure communication. Accordingly, designing and implementing new artificial chaotic systems have become an active topic of research.

Poincaré-Bendixson theorem implies the necessary condition for an autonomous continuous system to behave chaotically is at least 3-dimensional with at least one nonlinearity. Linear systems could not yield chaotic dynamics. However, in reality linear systems exist far and wide while chaos seems to only occur in rare specific circumstances. Does there exist a bridge to connect linear systems and chaos such that chaos phenomenon can be generated and observed as widely as what linear systems do? The answer is **YES**. In [4], we presented a new approach called chaos entanglement to achieve chaotic dynamics by entangling two or multiple **stable** linear subsystems.

To further explore the potential of chaos entanglement, in this paper, we study chaos entanglement with **unstable** linear subsystems. Different from entangling stable linear subsystems, the challenging problem here is how to guarantee the boundedness of the whole system which is a necessary condition for generating chaos. Firstly, a new entanglement function is presented. One can utilize it to entangle three identical 1-dimensional unstable linear subsystems to generate chaos, or entangle two unstable linear subsystems with different parameters and different dimensions, or even entangle a large number of unstable linear subsystems to form an artificial chaotic network. Furthermore, dynamical analysis shows that the entangled subsystems are bounded and all equilibra are unstable saddle points once chaos entanglement is achieved. In addition, numerical computation confirms that this system possesses one positive Lyapunov exponent, which implies chaos. Along this way, by different unstable linear subsystems and different entanglement functions, a variety of novel chaotic attractors have been created and abundant complex dynamics are exhibited. Our finding indicates that chaos entanglement could be utilized as a guideline to effectively create desired chaotic systems/networks for engineering applications.

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Impulsive Control and Synchronization of Spatiotemporal Chaos in Gray-Scott Model

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As an interesting and complex nonlinear phenomenon, chaos occurs in many natural systems, such as biology networks, electrical circuits, lasers, oscillating chemical reactions, fluid dynamics. Since the landmark work by Otti, Grebogi and Yorke, controlling chaos has become an important aspect of chaos theory. Recently, the method of impulsive control has gained renewed interest due to its applications in many areas such as orbital transfer of satellite, ecosystems management, and chaos synchronization for secure communication. It has been proved to be an effective method to stabilize the chaotic system.

Synchronization of chaotic systems is one of the most interesting and significant phenomena of chaotic systems, which has been widely used in secure communication. As there are so many results about the impulsive control of dynamic systems modeled by ordinary differential equations, it is natural to study the impulsive control of dynamic systems modeled by partial differential equations. In this talk, we investigate the impulsive control and synchronization of spatiotemporal chaos in Gray-Scott model[1]. Inspired by the idea in [2], a new pinning impulsive controller is designed to stabilize and synchronize the spatiotemporal chaos in Grey-Scott model. some stabilization and synchronization criteria are obtained to guarantee that the whole states of the Grey-Scott model can be forced to some desired states by placing the impulsive controllers on one state of the system at each impulsive instant. Numerical simulations are given to illustrate the effectiveness of the theoretical results.

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Continuous-time Random Walks, Fractional Diffusion and Non-local Operators: Applications to Physics, Finance, and Engineering (SS-RWFDNO)

Organizers:
Mark M. Meerschaert (Michigan State University)
Enrico Scalas (University of Eastern Piedmont, Basque Center for Applied Mathematics)

Diffusion and relaxation phenomena are at the foundation of many physical processes. They also occur in heterogeneous media where anomalies appear. Normal diffusion cannot explain the empirical findings. Among the proposals to describe anomalous diffusion and relaxation, continuous-time random walks and related fractional-calculus models are linear, even if the operators involved are non-local in space and involve memory in time. Similar methods can be used for the description of price fluctuations in financial markets. In this session, these models will be introduced, and some recent developments in the theory and practical applications to physics, finance, and engineering will be presented.

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Numerically efficient stochastic solution of the space-time fractional diffusion equation through Monte Carlo simulation of continuous-time random walks

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The space-time fractional diffusion equation

$$\frac{\partial^\beta}{\partial t^\beta} u(x,t) = D \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) \tag{1}$$
$$u(x,0^+) = \delta(x), \quad x \in \mathbb{R}, \quad t \in \mathbb{R}_+, \quad \alpha \in (0,2], \quad \beta \in (0,1]$$

and its generalization that includes a drift term, the fractional Fokker-Planck equation, can be solved taking the diffusive limit of uncoupled continuous-time random walks (CTRW) with Lévy α-stable distributed jumps in space and Mittag-Leffler distributed waiting times. This can be done efficiently exploiting transformation formulas to generate the jumps ξ_α and waiting times τ_β from independent uniform random numbers $u_i, v_i \in (0,1)$, $i = x,t$,

$$\xi_\alpha = \gamma_x \left(\frac{-\log u_x \cos\phi}{\cos((1-\alpha)\phi)} \right)^{1-\frac{1}{\alpha}} \frac{\sin(\alpha\phi)}{\cos\phi}, \quad \tau_\beta = -\gamma_t \log u_t \left(\frac{\sin(\beta\pi)}{\tan(\beta\pi v_t)} - \cos(\beta\pi) \right)^{\frac{1}{\beta}}, \tag{2}$$

where $\phi = \pi(v_x - 1/2)$ and γ_i are scale parameters; in the diffusive limit $\gamma_i \to 0$ with $\gamma_x^\alpha = \gamma_t^\beta$ [1]. We show some results on stochastic integrals driven by a CTRW and on their diffusive limits [2]. We conclude with recently published properties and applications of the transformation maps given by Eqs. (2), see Fig. 1 [3].

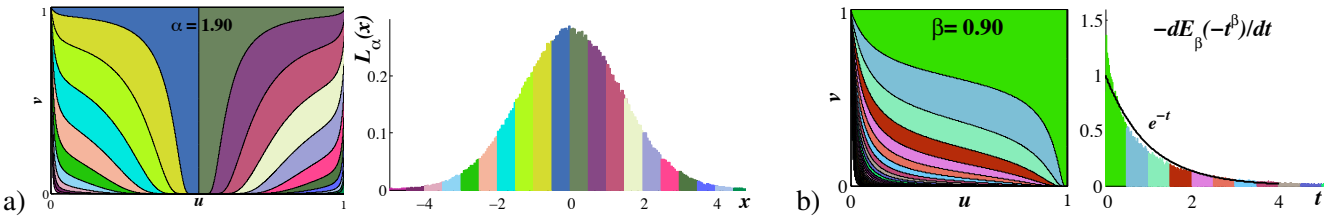

Figure 1: Transformation maps of Eqs. (2): a) Lévy α-stable jumps $\xi_\alpha(u,v)$ and b) Mittag-Leffler waiting times $\tau_\beta(u,v)$.

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CTRW Model for Fractional Wave Equations

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Fractional wave equations are important in many areas of science and engineering [3, 4, 5]. Fujita [2] proposed a stochastic solution to the time-fractional wave equation

$$\frac{\partial^y}{\partial t^y} p = \Delta_x p,$$

using the supremum of a negatively skewed stable process. The index $\alpha \in (1,2)$ of that stable process corresponds to a fractional time derivative of order $y = 2/\alpha$. In this talk, we present a continuous time random walk model for that same fractional wave equation. In the long time limit, this model leads to a stochastic solution involving the inverse or hitting time of a stable subordinator with index $1/\alpha$. The subordinator in our model is the first passage time of the stable process in Fujita [2], and its inverse is connected to the stable process of Fujita through the Zolotarev duality formula for stable densities [9], which also implies a space-time duality for fractional evolution equations [1]. The continuous time random walk model can be useful for particle tracking solutions to the fractional wave equation. These results complement some recent results of Meerschaert et al. [6] and Straka et al. [7] for the power law wave equation

$$\frac{1}{c_0^2}\frac{\partial^2}{\partial t^2} p + \frac{2\alpha_0}{c_0 b}\frac{\partial^{y+1}}{\partial t^{y+1}} p + \frac{\alpha_0^{2y}}{b^2}\frac{\partial^{2y}}{\partial t^{2y}} p = \Delta_x p$$

with $b = \cos(\pi y/2)$, a model for medical ultrasound.

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Applications of Random Renormalization Group Operators

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Many diffusive processes (such as Brownian motion, fractional Brownian motion, and α-stable Lévy motion) are fixed points of a renormalization group operator that relates a change in temporal scale with a corresponding change in spatial scale that obeys a power-law. We consider an alternative family of renormalization group operators where the power-law is treated as a random variable that may depend on the scale. Fixed points of these operators are, e.g., fractional Brownian motion with random Hurst exponent and α-stable Lévy motions with random stability parameter. Bayes' theorem is used to estimate the distribution for the power-law, which is then used to determine scaling laws. Applications to multiscale problems such as the sum of two of α-stable Lévy motions (with different stability parameters) and drifters in the Gulf of Mexico will be considered.

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Continuous-time Random Walk from a Continuous Double Auction

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We present a statistical model of the continuous double auction with zero-intelligence agents based on [1] and [2]. In our simplified model, only discrete prices from 1 to N are possible, limit orders and market orders are placed in unitary quantities and the order arrival process is described in terms of two independent $M/M/1$ queues [3]. The auction defines a continuous-time random walk for prices (or for logarithmic prices). We derive the conditions for the ergodicity of the auction and we study the effect on the price process. By means of Monte Carlo simulations and heuristic analysis, we show that there are three different regimes. In particular, in the ergodic regime, prices are unstable. We further study the limit of low traffic, where incoming limit orders immediately transform into market orders and a trade takes place. In this case, we can explicitly write the transition probabilities for the Markov chain of prices and compute its invariant measure. In the opposite limit of congested queues, the price randomly fluctuates between two adjacent values and the price process becomes an instance of the random telegraph process. Finally, we analyze the behavior of the average first passage time to 1 or to N for the price process by means of Monte Carlo simulations. A result of such simulations is shown in Figure 1.

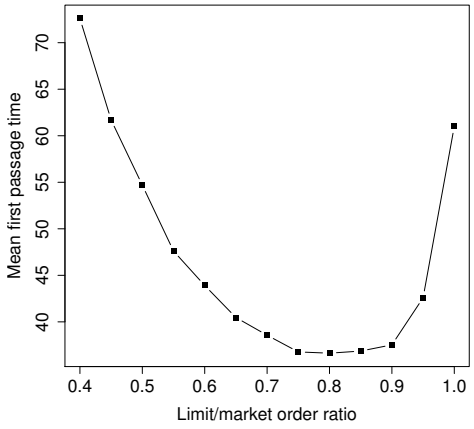

Figure 1: Average first passage time to either 1 or N as a function of the ratio between the arrival rate of limit orders and the one of market orders. In this simulation, $N = 40$ and the initial price is set to 20.

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Analysis for Nonlinear Equations Involving Space Fractional Diffusion

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We will describe recent results for integro-differential equations in the nonlinear setting with a fractional diffusion which has a jumping measure with strong spatial directional dependence, and even the situation where the directional dependence can change in a way which depends upon both the unknown function (hence nonlinear) and the current location in space.

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Correlation structure of fractional Pearson diffusions

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Fractional differential equations are an important and useful tool in many areas of science and engineering [1, 2, 3, 4, 5]. In a heterogeneous environment, the coefficients of the diffusion equation will naturally vary in space. Pearson diffusions form a tractable class of variable coefficient diffusion models with polynomial coefficients. The process $X_1(t)$ is called a Pearson diffusion if it solves the stochastic differential equation
$dX_1(t) = \mu(X_1(t))dt + \sigma(X_1(t))dW(t)$ with $\mu(x) = a_0 + a_1 x$ and $D(x) = \frac{\sigma^2(x)}{2} = d_0 + d_1 x + d_2 x^2$.

These processes include the Ornstein-Uhlenback process and the Cox-Ingersoll-Ross (CIR) process, which are used in finance. Their steady state distributions belong to the class of Pearson distrbutions. In a fractional Pearson diffusion, the time variable is replaced by an inverse α-stable subordinator independent of the process X_1 [6]. The resulting stochastic process is non-Markovian, but its one dimensional distributions are governed by the fractional Pearson diffusion equation, obtained by replacing the first time derivative in the Pearson diffusion equation with a Caputo fractional derivative of the same order $0 < \alpha < 1$ [7]. The purpose of this paper is study the correlation structure of fractional Pearson diffusions in steady state [8].

Theorem. Suppose that $X_1(t)$ is a Pearson diffusion in steady state, so that its correlation function is given by $\mathrm{corr}[X_1(s), X_1(t)] = \exp(-\theta|t-s|)$, $\theta > 0$, $t, s > 0$. Then the correlation function of the corresponding fractional Pearson diffusion $X_\alpha(t) = X_1(E_t)$, where E_t is the standard inverse α-stable subordinator independent of X_1, is given by

$$\mathrm{corr}[X_\alpha(t), X_\alpha(s)] = E_\alpha(-\theta t^\alpha) + \frac{\theta\alpha t^\alpha}{\Gamma(1+\alpha)} \int_0^{s/t} \frac{E_\alpha(-\theta t^\alpha (1-z)^\alpha)}{z^{1-\alpha}} dz \tag{1}$$

for $t \geq s > 0$, where $E_\alpha(z)$ is the Mittag-Leffler function.

It follows from the Theorem that fractional Pearson diffusions exhibit long-range dependence.

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Statistical Aspects of Environmental and Ecological Modeling (SS-SAEEM)

Organizers:
Vyacheslav Lyubchich (University of Waterloo)
Yulia R. Gel (University of Waterloo)
Chad Shouquan Cheng (Environment Canada)

The indubitable importance of preserving the safe and sustainable environment for current and future generations instigates an extensive number of interdisciplinary projects on biodiversity, climate change, ecology, etc., and as underlined by Mathematics of Planet Earth project (MPE), statistical science plays an increasingly profound role in such multidisciplinary research initiatives. This special session aims to highlight some recent advances and trends in statistical modeling of environmental and ecological processes, such as, for example, high dimensional data analysis, data visualization, nonparametric procedures, pattern recognition, risk assessment and forecasting in environmental sciences.

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Accounting for Temperature when Modeling Population Health Risk Due to Air Pollution

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The Air Health Indicator [1] is a joint Health Canada / Environment Canada initiative. A component in the indicator is an estimate of the time-dependent population health risk due to short-term (acute) effects of air pollution. The standard approach for this risk estimation uses a Generalized Additive Model framework [2, 3] which includes one or more air pollutants and one or more temperature terms as covariates, as well as a smooth function of time. In this risk modeling framework, the temperature is not the primary focus, but is included to ensure that common structure between the mortality (response), the pollutant(s), and the temperature is not included in the risk attribution.

Using tools from signal processing, spectrum estimation, and harmonic analysis, we analyze the smooth function link that is commonly used when including temperature. We show that for a single lag of temperature, the traditional *J*-, *U*-, or *V*-shaped relationship between temperature and mortality is largely a function of low-frequency mortality structure and is thus accounted for by the smooth function of time typically included in risk models. We further compare and contrast the first few primary lags of temperature, and demonstrate differences in their structure, especially with respect to "cold effects". We conclude with a discussion of the connection between this work and recent work on Distributed Lag Non-Linear Models [4], and of the differences in risk evident from choice of temperature inclusion.

Key words: population health risk, Generalized Additive Models, air pollution, temperature, dlnm

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Estimation of Absolute and Relative Abundance

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In the face of increasing extinction rates, it is vital to have estimates of relative and absolute species abundance and their relationship to important factors. For species that live in the oceans or large lakes, this can be a difficult task. Information on relative abundance of commercial fish stocks can be inferred from catch-per-unit-effort (CPUE). In this talk I will present a Bayesian model for trends in CPUE over time and the relationship between CPUE and important covariates. The model will be illustrated using spatial and temporal data on whitefish in the Canadian waters of Lake Huron from 1979 to 2010. It was found that CPUE has steadily decreased from a high in the mid-80's. I will also present a method for estimating abundance from a single binary acoustic time series. The dependence in the series is exploited to allow the estimation of abundance when some animals remain hidden, and in the face of uncertainty about the range over which sounds carry. Simulations show that the method can give reasonable estimates of absolute abundance in some settings. An extension to multiple time series will also be discussed. The method is illustrated using data on sperm whales in the Sargasso Sea.

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Changing stream flow augmented challenges: Modeling of water allocation policy for ecohydrological sustainability in Maine, USA

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Snowmelt driven steamflow variability and trends are extremely vital from the context of sustainable water allocation policy. The term sustainability has a lot of dimensions but in general that fulfill the current demand without hampering the future. Besides water allocation is a subtraction for the streams, and an addition to society, a stressor for floodplain ecology. Hence attaining sustainability in water allocation is a critical task and requires up to date policy. In general policy recommends the lower threshold for the stressors and capable of handling the augmented challenges for the changing future. For eco-hydrological sustainability, water allocation policy should be a threshold guideline that will ensure the stream health, ecological sustenance and maximum possible addition to the human society. State of Maine has adopted the seasonal aquatic base flow (SABF) as the key policy threshold for the allocation of B type and lower graded streams. Scrutinizing the variability in stream flow can act as a hub that conveys the implication of the ecological responses and also footprint of the changes in the climate. The analysis will affords to figure out significant trends and their insight in seasonality, magnitude, timing, duration and frequency in stream flow. A proper assessment of the SABF in Maine's stream is the key to justify the water allocation policy from the context of eco-hydrological sustainability. A Range of Variability Analysis (RVA; Richter et. al. 1997) has been adopted to quantify the indicators and degree of alteration resulting from the implementation of water allocation policy. The alterations of individual indicators over the watershed are capable of interpreting many aspects of the linkages from eco-hydrology to the sustainability of the water allocation policy. Some augmented challenges from the changing stream flow in implication of the policy have also been explored.

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Analyzing inter-annual variability in North American net ecosystem CO_2 exchange

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Recent *in situ* studies have documented that rising Arctic air temperatures have both increased atmospheric effluxes of CO_2 from thawing permafrost, and enabled northward movements of the shrub and tree lines, leading to increased uptake of atmospheric CO_2 by vegetation. Understanding changes over time in Arctic net ecosystem CO_2 exchange (NEE) is crucial since the response of the northern carbon cycle to climate change will influence future levels of atmospheric CO_2 [1]. However, although atmospheric concentrations of CO_2 can be measured globally, NEE can only be measured *in situ* over $<$1km areas. Regional estimates of NEE are therefore generated using a model approach.

The Polar Vegetation Photosynthesis Respiration Model (PolarVPRM) was developed to generate estimates of high-latitude NEE using remotely sensed observations. Respiration (R) is estimated as a linear function of air temperature (T_a) during the growing season ($R = \alpha T_a + \beta$), and as a linear function of soil temperature (T_s) during the snow season ($R = \alpha_s T_s + \beta_s$). Photosynthetic uptake of CO_2 is calculated according to remote sensing observations of the fraction of photosynthetically active radiation available for absorption by vegetation, and estimates of the influence air temperature, water availability and leaf phenology have on the rate of photosynthesis. Parameters describing the relationships between land surface variables are calibrated using *in situ* measurements of NEE and site meteorology. Validation indicated a good fit between PolarVPRM estimates of NEE, and *in situ* observations of NEE collected at non-calibration sites.

Inter-annual variability in PolarVPRM estimates of NEE and its drivers over North America (55–83°N) can provide important insights into the response of the high-latitude carbon cycle to recent (2001–2012) climate variability. The Theil-Sen approach was applied to each $\frac{1}{6}^\circ \times \frac{1}{4}^\circ$ pixel in order to examine the median slope of changes over time in the high-latitude carbon cycle and its drivers. Findings indicated that tundra regions are likely to be releasing CO_2 at an increased rate due to warming soil and air temperatures. Tundra vegetation appears to be undergoing an increase in CO_2 uptake due to warming temperatures and increases in remotely sensed vegetation indices, whereas forests tend to be uptaking less CO_2 over time. Overall, high-latitude ecosystems appear to be uptaking substantially less carbon each year in response to climate-driven shifts in land surface and meteorological influences on NEE.

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Testing for synchronism among trends in environmental data

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The climate change brings increasingly more alterations and permanent impact on all aspects of human life and welfare. Hence, it is of particular interest to investigate how trends in climatic variables, for example, such as precipitation and temperature, are related to each other and to study their association with dynamics of various ecological, geological, economic and socio-demographic factors. For example, aligning climatic trends with actuarial information is one of the major concerns for insurance companies, while detection of joint trends in lake freeze-up and break-up timings is directly related to sustainability of fishing industry.

In this talk, we explore a new statistical test for synchronism of trends exhibited by multiple time series, i.e., testing whether two or more time series follow the same common trend. The core idea of our new approach is based on employing the local regression goodness-of-fit test [1] – [3], which allows to detect possibly non-monotonic (non)linear trends. We illustrate the proposed methodology by simulations and case studies on assessing joint dynamics of various climatic variables in space and time.

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Censored Gamma Regression with Applications

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Most types of data are what we term as complete data. Complete data means that the value of all the observations are known or observed. In many cases, the value of some sample unit is unobserved means the observations are known only to fall below a censoring point but we do not know by how much. Data containing such uncertainty as to exactly when the event happened is termed as left censored data. This presents difficulties in statistical analysis of the data. In this talk, we propose a new model for the left-censored data under the assumption that the underlying distribution is gamma.

We examine methods for estimating and fitting the parameters of the left-censored gamma data such as, maximum likelihood estimation. Many types of environmental data are left-censored. In water quality, parameters such as pH, phosphates, nitrates, nitrites and many others are only determined for values that exceed some lower threshold limit, δ. We use our proposed model with the forest fires data from the Montesinho Natural Park from January 2000 to December 2003. In our data, the output variable is the total area burned in each of 517 forest fires in a three year period in a large natural park. When this area is less 0.01 ha, it was recorded as 0 and so was effectively left censored with $\kappa = 0.01$ ha. We assume that the distribution of fires is from a left-censored gamma distribution. We have demonstrated that using a gamma regression with left-censoring outperforms linear regression using a logarithmic transformation. For other types of data, we have found that a shifted gamma distribution may improve the fit.

Statistical Data Analysis and Geometry (SS-SDAG)

Organizers:
Shoja Chenouri (University of Waterloo)
Paul Marriott (University of Waterloo)

This session is dedicated to statistical data analysis and modelling through geometric concepts, and looks at ways that geometry and statistics can inform each other. Traditionally, statistical methods assume that data lies in linear subspaces of some ambient Euclidean space. However, in many application problems,in fact it lives in non-Euclidean spaces, and therefore should be naturally modelled on manifolds, or other geometric objects. The goal of this session is to bring together statisticians who study or apply geometric tools, and those who have a general interest in applied geometry.

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The Application of the Convex Geometry in the Generalized Method of Moments for Mixture Models

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To fit a finite mixture model with known order, there are many existing estimation methods, including the method of moments (MM) [1], the maximum likelihood estimator (MLE) [2], the non-parametric maximum likelihood estimator (NPMLE) [3]. The generalized method of moment (GMM) for mixture models is proposed as a new method for fitting a mixture model with known order. In this talk, we will see the role that convex geometry play in developing this new estimation method for mixture models. First of all, the GMM estimator is considered in the moment space, which is a low-dimensional approximation of the likelihood space. Such approximation increases the efficiency of the estimator when compared to the MM. Secondly, the GMM estimator is under a convex optimization framework, which can be computed fast and easily. Therefore, the GMM estimator has computational advantages over the MLE, which is usually obtained by the gradient based algorithms or the EM-algorithm. Lastly, the GMM estimator considers the boundary properties of the feasible region. This makes the new estimator more likely provide a model with given order than the NPMLE.

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Robustness in dimensionality reduction

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Many popular dimensionality reduction methods are considered to be highly sensitive to outliers, and some robust procedures are proposed without a general and well-established criterion. We extend several classical concepts (both local and global) to measure and compare the robustness of the dimensionality reduction methods (both linear and non-linear). Measures concerning the local and global topology preservation are defined as badness criterion, and based on these measures, the performances of different types of methods are assessed under contaminated dataset or misspecified model. Also, we consider the estimation of intrinsic dimensionality and the effect of outliers on this estimation.

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Computational Aspects of Inference in Local Mixture Models (LMM)

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Local Mixture Models give an inferentially tractable but still flexible alternative to full mixture models. The parameter space naturally includes boundaries of different sorts. These boundaries mean that computing the maximum likelihood estimate (MLE) is not standard. This talk shows how the geometry of ruled and developable surfaces enable fast and efficient algorithms for finding the MLE to be developed.

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Spanifold: Spanning Tree Flattening Onto Lower Dimension

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Dimensionality reduction and manifold learning techniques attempt to recover a lower dimensional submanifold from the data as encoded in high-dimensions. Suppose $\mathbb{M}$ is a Riemannian manifold of dimension d embedded in $\mathbb{R}^D$, where $d < D$, and that $\mathbb{M}$ can be topologically embedded in a linear subspace of dimension d. Such an embedding can typically be constructed by unfolding the manifold with some possible distortion of the geometry.

Standard methods, such as Isomap and LLE, map the high dimensional data points into low dimension so as to globally minimize a so-called energy function, which measures the mismatch between the precise geometry in high dimensions and the approximate geometry in low dimensions. However, the local effects of such minimizations are often unpredictable, because the energy minimization algorithms are global in nature. In contrast to these methods, the Spanifold algorithm of this paper constructs a tree on the manifold, and flattens the manifold in such a way as to approximately preserve pairwise distance relationships within the tree. The vertices of this tree are the data points, and the edges of the tree form a subset of the edges of nearest neighbour graph on the data. In addition, the pairwise distances between data points close to the root of the tree undergo minimal distortion as the data are flattened. This allows the user to design the flattening algorithm so as to approximately preserve neighbour relationships in any chosen local region of the data.

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Quantifying the Asymptotic Coverage Probabilities of Bootstrap Confidence Regions

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Abstract

When the unknown parameters are on or close to the boundary of parameter space, the classical methods may not give confidence regions for the unknown parameters with asymptotically correct coverage probabilities. The bootstrap methods are intuitively in favour as an alternative. In this talk, we quantify the asymptotic coverage probabilities of two types of bootstrap confidence regions: bootstrap percentile confidence region and bootstrap likelihood ratio confidence region. We show that the asymptotic coverage probability of the first type is always above the nominal level, while that of the second type can be below or above the nominal level. We further propose a method to construct confidence region with asymptotically correct coverage probability.

Structured Graph Theory (SS-SGT)

Organizers:
Kathie Cameron (Wilfrid Laurier University)
Chinh Hoang (Wilfrid Laurier University)

Many problems that are NP-complete for arbitrary graphs can be solved in polynomial time when restricted to special classes of graphs. The polynomial-time algorithms typically exploit the structures of these graphs. In this session, we present recent results in this direction.

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Completing colored graphs to meet a target property

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We consider the problem of deciding whether a properly k-colored graph can be completed (by adding edges while maintaining a proper coloring) to have a given property. When k is *not* fixed, we show the problems of deciding whether a k-colored graph can be completed to be a circular-arc graph, a proper circular-arc graph, and a unit circular-arc graph are NP-complete. Then, we provide a complete classification of the complexity of the circular-arc colored graph completion problem when the number of colors used is fixed. Specifically, given a k-colored graph, we show that when $k = 2$, there is an $O(n)$ time algorithm for the problem, but when $k = 3$, the problem is NP-complete; in turn, the problem remains NP-complete for every fixed k, $k \geq 3$. We provide an identical classification for the problem of completing a k-colored graph to be a Helly circular-arc graph. We show that the problems of deciding whether a 3-colored graph admits a unit circular-arc completion and a proper circular-arc completion are also NP-complete. To the best of our knowledge these are the first instances of a colored graph completion problem on 3-colored graphs that are hard. We also show that deciding whether a 3-colored graph admits a strongly chordal completion can be decided in $O(n^2)$ time; our algorithm is based on a characterization of bi-connected 3-colored graphs that admit a strongly chordal completion. It is known that the sandwich problems for interval and circular-arc graphs are NP-complete. It follows from our results that the sandwich problem for Helly circular-arc graphs is NP-complete.

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Coloring graphs without induced paths of fixed lengths

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Let P_t denote the induced path on t vertices. It is known that the coloring problem for P_5-free graphs is NP-hard. However, for a fixed $k \geq 3$, there is a polynomial time algorithm to k-color a P_5-free graphs. One may wish to determine the complexity of k-coloring P_t-free graphs for other values of k and t. We survey recent results in this direction.

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Constructions of k-critical P_5-free graphs

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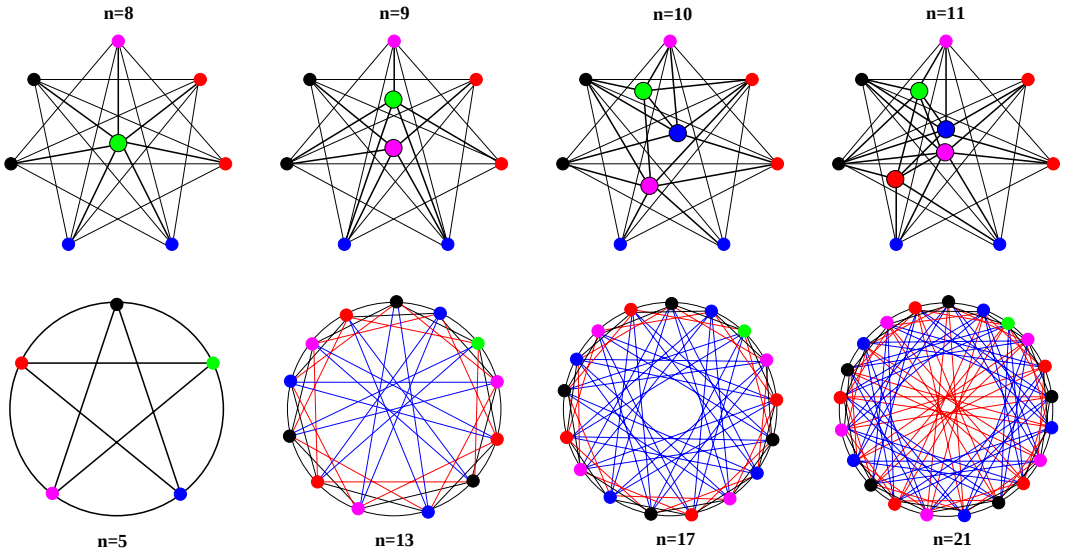
With respect to a class $\mathcal{C}$ of graphs, a graph $G \in \mathcal{C}$ is said to be *k-critical* if every proper subgraph of G belonging to $\mathcal{C}$ is $k-1$ colorable. We construct an infinite set of k-critical P_5-free graphs for every $k \geq 5$. We also prove that there are exactly eight 5-critical $\{P_5, C_5\}$-free graphs as follows:



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On Hendry's conjecture on cycle extension

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Hendry conjectured in 1990 that for a non-Hamiltonian cycle C in a Hamiltonian chordal graph, there exists a cycle C' such that $V(C) \subseteq V(C')$ and $|V(C')| = |V(C)| + 1$; the conjecture is open. A *spider* is a subdivision of a $K_{1,r}$, $r \geq 0$. A *spider intersection graph* is the intersection graph of subtrees of a spider. We prove Hendry's conjecture for the class of spider intersection graphs. This result extends previously known results for interval graphs and split graphs.

Symmetry in Nonlinear Dynamics: Theory and Applications (SS-SNDTA)

Organizers:
Manuele Santoprete (Wilfrid Laurier University) and Ray McLenaghan (University of Waterloo)

Symmetry is often found in dynamical models of physical or biological phenomena. This scientific session will focus on recent advances in theoretical and applied aspects of nonlinear dynamics where symmetry plays an important role.

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Integrable Viscous Conservation Laws

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We propose an extension of Dubrovin's perturbative approach to the study of normal forms for non-Hamiltonian integrable scalar conservation laws. The explicit computation of the first few corrections leads to the conjecture that such normal forms are parametrized by one single functional parameter, named viscous central invariant.

A constant valued viscous central invariant corresponds to the well-known Burgers hierarchy. The case of a linear viscous central invariant provides a viscous analog of the Camassa-Holm equation, that formerly appeared as a reduction of a two-component generalization of the Camassa-Holm equation. We write explicitly the negative and positive hierarchy associated with this equation and prove the integrability showing that they can be mapped respectively into the heat hierarchy and its negative counterpart, named Klein-Gordon hierarchy.

A local well-posedness theorem for periodic initial data is also proven and some numerical simulations are presented. Finally, we explicitly construct asymptotic solutions obtained by quasi-Miura transformations and discuss Dubrovin'ss Universality conjecture for the local behaviour of the solutions near the point of gradient catastrophe.

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An obstruction class for isotropic fibrations

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A classical theorem due to Birkhoff states that an invariant, essential curve of a twist map of the annulus is a graph. Bialy and Polterovich generalize this result in higher dimensions: If F is a Lagrangian submanifold invariant by an "optical" Hamiltonian diffeomorphism A such that $A|F$ is chain-recurrent, then F is a graph iff its Maslov cycle vanishes [2, 3]. Arnaud has recently given a proof that uses weak KAM theory [1]. I will discuss how these ideas may be applied to understand when an invariant, isotropic submanifold is a graph and give applications to non-commutatively integrable Hamiltonian systems.

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Relative Equilibria and Rotopulsators of the Curved N-Body Problem

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We consider the motion of N point particles in spaces of constant curvature, namely on the sphere $\mathbf{S}^3$ and on the hyperbolic sphere $\mathbf{H}^3$, [6, 7]. We first prove some criteria for the existence of relative equilibria and rotopulsators and then use them to find large classes of such solutions, [1, 2, 3, 4, 5].

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A New Approach to the Integrability of the Suslov Problem

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We develop a new approach to the integrability of a generalized Klebsh–Tisserand case of the Suslov nonholonomic rigid body problem. We use the Poincaré–Hopf Theorem to prove that, under certain conditions, the genus g of the compact sets of integrals of motion is given by $g = 1 + n$, where $0 \leq n \leq 4$ is the number of connected components of the kernel of the multiplier f (the known function that transforms the Suslov problem to Hamiltonian form after the reparameterization of time $d\tau = f(q)\,dt$, where $q \in Q$, the configuration space of the system).

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Saari's homographic conjecture for the planar equal-mass three-body problem under the Newton potential and a strong force potential

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In 2005, D. Saari formulated his homographic conjecture for N-body problem as follows [5, 6]; for the N-body problem under the homogenious potential $U = \sum m_i m_j / r_{ij}^{\alpha}$, $\alpha > 0$, the configurational measure $\mu = I^{\alpha/2} U$ is constant if and only if the motion is homographic. Here, m_i $(i = 1, 2, \ldots N)$ is mass for the body i, r_{ij} is the mutual distance between the body i and j and $I = \sum m_i m_j r_{ij}^2$ is the moment of inertia.

For the three-body problem, the only two types of homographic motion exist, namely, the Euler's collinear solution and the Lagrange's equilateral triangle solution.

In 2008, F. Diacu, T. Fujiwara, E. Pérez-Chavela and M. Santoprere showed that this conjecture is true for large set of initial conditions for planar three-body problem [1, 2]. They derived a condition which must be satisfied if a non-homographic planar motion with constant configurational measure exist. Then, they showed that the condition is failed to be satisfied by many cases of initial conditions.

In 2012, T. Fujiwara, H. Fukuda, H. Ozaki, and T. Taniguchi proved the conjecture for the planar equal-mass three-body problem under a strong force potential($\alpha = 2$) [3] and the Newton potential($\alpha = 1$) [4].

To prove the conjecture for these cases, we used the symmetry under the permutations of three-bodies [4]. This symmetry make our proof simple. We will review how this symmetry work in our proof of the Saari's homographic conjecture.

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Symplectic Semiclassical Wave Packet Dynamics

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I will talk about the geometry and dynamics of semiclassical wave packets of Heller [1] and Coalson & Karplus [2]. The semiclassical Gaussian wave packet

$$\psi(x) = \exp\left\{ \frac{i}{\hbar}\left[\frac{1}{2}(x-q)^T \mathscr{C}(x-q) + p\cdot(x-q) + (\phi + i\delta) \right] \right\}$$

is an ansatz for the Schrödinger equation that provides a description of the transition regime between quantum and classical mechanics. The parameters (q,p,ϕ,δ) are in the space $T^*\mathbb{R}^d \times \mathbb{S}^1 \times \mathbb{R}$ with d being the dimension of the physical space, whereas $\mathscr{C} = \mathscr{A} + i\mathscr{B}$ is a $d \times d$ complex symmetric matrix with a positive-definite imaginary part, i.e., the matrix $\mathscr{C}$ is an element in the *Siegel upper plane* defined by

$$\Sigma_d := \left\{ \mathscr{C} = \mathscr{A} + i\mathscr{B} \in \mathbb{C}^{d\times d} \mid \mathscr{A}, \mathscr{B} \in \mathrm{Sym}_d(\mathbb{R}),\, \mathscr{B} > 0 \right\},$$

where $\mathrm{Sym}_d(\mathbb{R})$ is the set of $d \times d$ real symmetric matrices, and $\mathscr{B} > 0$ means that $\mathscr{B}$ is positive-definite.

I will show how to formulate the dynamics of semiclassical wave packets from the symplectic-geometric point of view by exploiting the geometric structure of quantum mechanics; this approach effectively "strips away" quantum effects from quantum mechanics and incorporates them into the classical description of mechanics. This extends the work of Faou & Lubich [3] and Lubich [4] for the "spherical" case, i.e., $\mathscr{C} = (a+ib)I_d$ with $a \in \mathbb{R}$, $b > 0$, and I_d is the identity matrix of size d.

The dynamics of the semiclassical wave packets has an $\mathbb{S}^1$-symmetry, and reduction by the symmetry reveals a simplified symplectic structure that is closely related to the symplectic structure of the Siegel upper plane Σ_d, which is in fact a homogeneous space $Sp(2d,\mathbb{R})/U(d)$, where $Sp(2d,\mathbb{R})$ is the symplectic group of degree $2d$ over real numbers and $U(d)$ is the unitary group of degree d. This point of view provides a geometric interpretation of the Hagedorn wave packet [5].

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Orthogonal separation of the Hamilton-Jacobi equation on Spaces of Constant curvature

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The talk will present a theory of orthogonal separation of the Hamilton-Jacobi equation on spaces of constant curvature, with examples in Euclidean space. The theory is based on results of Eisenhart [Eis34], which connect orthogonal separation of the Hamilton-Jacobi equation to the existence of special types of Killing tensors known as characteristic Killing tensors.

We use geometrical properties of Killing tensors to classify separable webs and develop an algorithm to separate the Hamilton-Jacobi equation. In particular, our solution method involves a recursive classification of characteristic Killing tensors by way of the warped product decompositions [Nol96] of the Riemannian manifold they induce. This classification is built up on Benenti's theory of a special but important class of characteristic Killing tensors [Ben92, Ben04, Ben05].

The method has been successfully applied to Euclidean space and the n-sphere; in this case, other authors have arrived at this solution using other methods [WRW03]. We will present some examples of this method for well known Hamiltonians in 3-dimensional Euclidean space. Current work involves applying the method to Hyperbolic, Minkowski and de Sitter space. In addition to being a viable method for solving Hamilton's equations for some existing natural Hamiltonians, this method allows us to find new integrable systems defined on these spaces as well.

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Orbits in the Symmetric Four-body Problem

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The gravitational N-body problem has long been a source of theoretical investigation with application to astronomical systems. There is a rich and varied dynamics. With systems of four bodies arranged symmetrically, the symmetry tends to reduce the complexity of the system so that it is perhaps more similar to one with three bodies. Although, such systems also provide a starting point for our understanding of more general four-body systems.

In the three-body equal-mass case a simple collinear periodic orbit was discovered by Schubart in 1956 [1]. Similar orbits extend to the plane [4], and unequal masses [2, 3], and also exist for the four-body problem [5]. Included within this talk we will look at some orbits of this general nature.

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Traveling Waves and Conservation Laws for Complex mKdV-type Equations

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For a class of U(1)-invariant complex mKdV equations we present traveling waves and conservation laws containing the known integrable generalizations of the real mKdV equation. Complex solitary waves and kinks that we derived generalize the well-known mKdV sech and tanh solutions. When computing explicitly all first-order conserved densities we obtained phase-invariant counterparts of the mKdV conserved densities for momentum, energy, and Galilean energy, and a new conserved density describing the angular twist of complex kink solutions.

For both, the symmetry and the conservation law computations, remarks about the computational challenges in solving a non-linear ODE system and in dealing with many jet-variables in large overdetermined systems are made.

Simulations in Soft Matter and Molecular Bio-Physics (SS-SSMMBP)

Organizer:
Cristiano L. Dias (New Jersey Institute of Technology)

Computer simulations are playing an important role in our understanding of soft matter and molecular Bio-Physics. In recent years we have seen tremendous progress in these areas motivated by advances in supercomputers and simulation techniques. This special session will bring together scientists developing new computational methods in soft matter and scientists using conventional techniques to study emerging phenomena in molecular Bio-Physics. The goal will be to foster interactions between method development in soft matter and potential applications in molecular Bio-Physics.

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Colloidal disks in nematic liquid crystals under the action of magnetic fields

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We simulated magnetic disks immersed in a liquid crystal using a lattice-Boltzmann algorithm modified for liquid crystals. In the absence of external torques, disks with homeotropic anchoring align with their surface normal $\bar{a}$ parallel to the director of the nematic liquid crystal $\bar{n}$. In the presence of a weak magnetic field (<10G) the disks will rotate to equilibrate the magnetic torque and the elastic torque due to the distortion of the nematic director. When the magnetic field rotates the disks so that $\theta = (\widehat{\bar{n}\,\bar{a}})$ becomes greater than $\frac{\pi}{2}$, the disks will go through the transition in which $\theta \to \pi - \theta$. The analysis of defects in the nematic liquid crystal during the described above rotation was performed.

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Coarse-Grained Atomistic Modeling of Colloid Crystallization and Glass Formation with Phase Field Crystal Methods

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[3] *McGill University, Montreal, Canada*

Phase Field Crystal (PFC) models [1, 2] have been used to study a variety of phenomena in traditional atomic materials such as metals and metal alloys, but the same basic framework has also been applied to soft materials such as colloidal suspensions, liquid crystals, and polymers. Such models simulate long time scale diffusive dynamics at the 'atomic' level by coarse-graining the rapid vibrational or Brownian movements into a time-averaged continuum number density field, as in classical density functional theory. One can then employ a coarse-grained time step close to the order of the characteristic diffusion time rather than the characteristic vibrational time. In this talk, the current state of PFC modeling of soft materials will be briefly outlined, with a particular focus on freezing and the dynamics of glass formation in simple model colloidal systems. Monodisperse and bidisperse suspensions will be discussed, and some minimal features of a successful PFC model for glass-formation outlined. These features lead to dynamics consistent with a fragile transition and the central predictions of mode-coupling theory. A physically-motivated time scaling results in qualitative agreement with basic glass transition phenomenology and experimental data across 12 orders of magnitude in time [3].

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The role of PEGylation in drug delivery: what can molecular dynamics simulation tell us?

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PEGylation, the attachment of poly(ethylene glycol) (PEG) to drug molecules or nanoscale drug delivery devices (nanovectors), is well established as a technique to create a "stealth sheath" that prologues bloodstream lifetime, hence efficacy. The most well developed nanovector, the only such treatment that is currently FDA approved, is the PEGylated liposome. PEGylation has been extremely successful, however considerable room for improvement remains; PEGylation increases the time drug delivery liposomes circulate in the bloodstream from $\sim$ 1 hour to the range of 1-2 days [1], however blood platelets, red blood cells, and some antibodies have a blood plasma circulation time in the range of months. For this reason several alternative polymers to PEG are currently under consideration [2]. A rational design approach to alternatives to PEG can only be followed if one has a good understanding of the specific properties of PEG, its structure in relation to the drug or nanovector to which it is attached, and its interaction with the bloodstream. Molecular dynamics simulation, using an all atom model, allows us to gain an atomic resolution picture of these systems, providing insight that is not attainable experimentally. Using molecular dynamics simulation, we have studied the surface of a PEGylated liposome, studying the effect of membrane state (gel or liquid crystal) [3] , presence of cholesterol in the membrane, density of PEG lipid [4], and targeting ligands expressed on the PEGylated liposome exterior [5]. We have also studied PEGylated drugs [6], both how the drug interacts with PEG, and how PEGylation of the drug affects the penetration of drugs into the cell membrane. In all of these studies, we have found that the specific properties of PEG, its solubility in both polar and non-polar solvents, and its acting as a polymer electrolyte, have a significant effect when used in drug delivery.

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Principles of Protein Folding from Coarse-Grained Modeling

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The so-called Levinthal paradox of protein folding is often understood as merely stating that folding by a completely random conformational search is impossible. This perception overlooks an important historical context of Levinthal's question, which was mainly a reaction to the fundamental theoretical implications of the experimental discovery of two-state, switch-like cooperative folding in the late 1960s [1]. The conceptual relationship between the origin of the Levinthal paradox and the notion of a funnel-like energy landscape will be discussed [2]. Comparisons between theory and experiment indicate a prominent role of desolvation barriers in cooperative folding [3]. These barriers narrow the range of attractive interactions. They contribute to an apparent general organizing principle involving a coupling between local conformational preferences and nonlocal packing interactions. Examples will be highlighted to illustrate how important folding principles have been gleaned from native-centric models of proteins [4], how nonnative interactions may be treated perturbatively [5, 6, 7], and how coarse-grained modeling has been used to predict/rationalize experimental observations [2]. Consistent with recent single-molecule FRET experiments [8], simulated folding transition path time in our coarse-grained chain models correlates only weakly with overall folding time. We found that this behavior as well as the distribution of transition path times can be essentially captured by a simple diffusion picture of folding. We found further that in our model, conformations in the initial stages of transition paths tend to form more nonlocal contacts than typical conformations with the same number of native contacts. This predicted statistical bias suggests that certain orderings of kinetic events with early nonlocal contact formation are preferred in productive folding [9]. Ramifications of these findings on protein folding theory will be explored.

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Nano-scale Dimer Motor in a Chemical Gradient

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Molecular machines, unlike macroscopic machines, operate in an environment with strong thermal fluctuations. A molecular motor, to counteract thermal motion and achieve propulsion, draws energy from its environment, e.g., chemical energy in the case of synthetic chemical motors [1]. Previous work includes the study of the dynamics [2] and the collective behaviour [3] of self-propelled sphere-dimer motors of meso-scale size.

We present a dimer motor of nanometer size in solvent, and analyze its motion using molecular dynamics. The solvent is treated explicitly, preserving both hydrodynamic and structural effects. The dimer is composed of a smaller catalytic (C) and a larger non-catalytic (N) sphere. The catalytic sphere catalyses the reaction of fuel (A) particles of the solvent to product (B) particles. This reaction produces a chemical gradient, where the concentration of product particles around the non-catalytic sphere is higher on the side facing the catalytic sphere, and lower on the other side. All constituents of the system interact via the short-ranged repulsive Weeks-Chandler-Andersen potential, with varying strength $\varepsilon_{\mathrm{NB}}$ for the interaction of non-catalytic sphere and product particles, and unit ε otherwise, which causes a spatial asymmetry of forces acting upon the non-catalytic sphere.

Despite the small size of the dimer relative to the solvent particles, and thus the strong thermal fluctuations, we measure directed motion of the dimer. We discuss the propulsion (Fig. 1) for various dimer sizes and interaction strengths, and the orientational auto-correlation. We analyse the short- and long-time dynamics using the mean-square displacement, and derive a formula based on the decay of velocity and orientational fluctuations.

The molecular dynamics simulations of 10^5 particles were conducted using a self-written parallel code. The program employs the OpenCL computing language [4] and the LuaJIT just-in-time compiler [5], resulting in a compact, efficient and adaptable simulation code for heterogeneous computers with a multi-core CPU and a GPU.

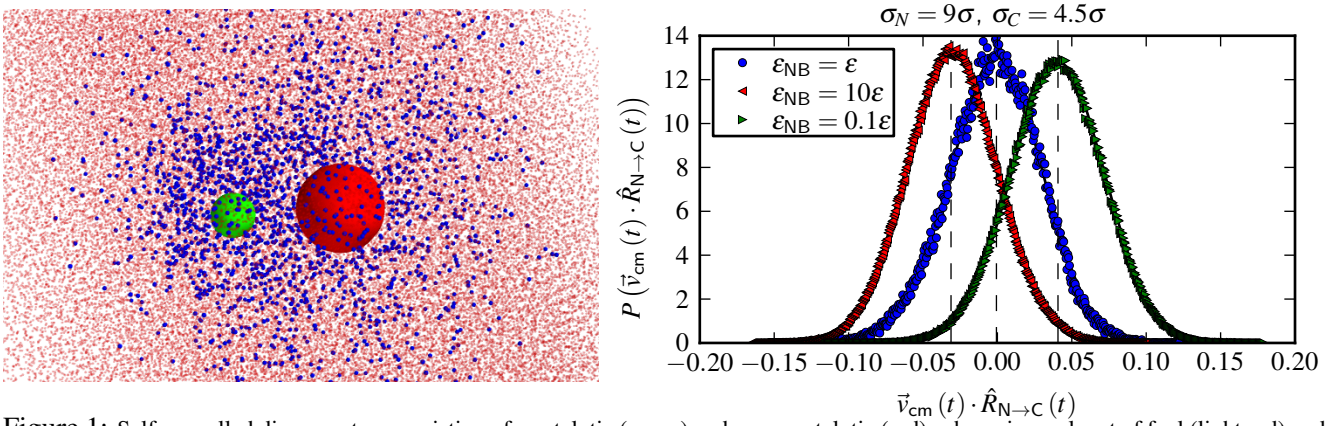

Figure 1: Self-propelled dimer motor, consisting of a catalytic (green) and a non-catalytic (red) sphere, in a solvent of fuel (light red) and product (blue) particles. The velocity of the dimer is projected onto its axis, and histogrammed over time and multiple realisations. The dimer exhibits a significant forward ($\varepsilon_{\mathrm{NB}} = 0.1\varepsilon$) or backward ($\varepsilon_{\mathrm{NB}} = 10\varepsilon$) propulsion in the presence of a chemical gradient.

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Unraveling the role of solvent-macromolecule interactions in determining the conformations of macromolecules in bulk, droplet and vacuum environments

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Liquid nanodroplets with excess charge are indispensable intermediates in electrospray ionization (ESI) techniques. ESI is often used to carry biological macromolecules from the bulk solution into the gaseous state via charged droplets. The droplets contract through evaporation of the solvent and a sequence of fission events involving charged species. Critical question in the ESI applications is how the conformations and charge states [1, 2, 3, 4] of macromolecules in the bulk is related to that in the droplet and the later gaseous state form [1]. The objective of the presentation is to address the relation of the conformations of macromolecules in the various settings utilizing molecular simulations. Sodiated poly(ethylene glycol) (PEG) in water is used as a prototype system because aqueous PEG has been studied extensively in ESI experiments and it has also been reported that PEG molecules in aqueous bulk solution demonstrate solvation properties similar to those of proteins in water. The PEG conformations in bulk were sampled by using the multiple replica repulsion (MRR) [5] technique and in vacuum by using replica exchange molecular dynamics. The MRR technique allowed us for the first time to observe directly emulsification of macromolecules at high salt concentrations. We found that PEG is released from sodiated aqueous droplets in a stretched conformation because of the large number of ions associated with the oxygen sites of PEG. These conformations do not reflect the conformations in the bulk solution.

The presented topic is of broad scientific interest among the scientists who work in the fields of electrospray mass spectrometry, aerosols, interactions of biological macromolecules with solvent and ions. The topic also partially overlaps with the field of polyelectrolytes. The assembled body of knowledge that we obtain through the systematic study of these problems will provide means to construct detailed theory to generalize the findings and lay the theoretical foundation for processes that give rise to the signals in the electrospray mass spectrometry methods. These studies assist in the understanding of macromolecule-solvent interactions.

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The implication of stochastic resonance effects on neurological disease quantifications

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Over last couple of decades, study of stochastic resonance (SR) phenomena has played a significant role in many real physical systems in order to extract input information in a noise-assisted environment (see Refs. [1, 2]). In addition to previous work, we present an application of stochastic resonance in a data-driven nonlinear bi-stable system, in which inhibitory and excitatory neuronal activities in the pre-frontal cortex (PFC) are quantified in healthy and disease model rodent brains.

Electrophysiological spiking activity of PFC neurons in the animal (rodent) model was recorded using multichannel, in-vivo 'tetrodes' at baseline (no pharmacological intervention), and with amphetamine (AMP) stimulation in the presence and absence of a GABAergic inhibitor, picrotoxin. Recordings were made pre-injection and then at 15, 60 and 180 minutes after. An adaptive multivariate empirical mode decomposition protocol was applied for processing and analyzing these non-linear and non-stationary data. Within the different experimental conditions, we parameterized both symmetric and asymmetric types of bi-stable model potentials through non-linear regression fitting (see Ref. [3]). In order to obtain functional patterns of neuronal dynamics in both control and disease states, we further characterized brain activity in the form of SR by applying the nonlinear Duffing oscillator model with respective shapes of parameterized potentials.

Increased GABAergic synaptic abnormalities and loss of dopamine fiber density in the disease model brain may increase energy barrier of potential wells and reduce the noise source that is inherent to the disease state neuronal network. These may simplify resonance effects, forming independent limit cycles in dynamic phase space, which may be a result of a reduction of dopaminergic (DA) neuronal activities in PFC in the disease state. In presence of excitatory type stimulation (amphetamine) the altered baseline DA activity may show non-bifurcating dynamic states in phase space. These may help to characterize dopamine agonist and/or antagonist activities in our bistable oscillator model and an inability to demonstrate information flow in the disease model brain.

Our analyses on spatio-temporal aspects of neuronal dynamics suggest that spontaneous neuronal activity, resulting from internally driven neuronal network force (such as synaptic connectivity) and source of physical noise, may provide asymmetries in our bi-stable model potential that has a strong influence on SR effect in order to quantify bi-stable brain dynamic phase transitions. Further quantification of dynamic multi-stabilities and corresponding phase transitions among different phases may correlate abilities of decision making in PFC, which may be absent in the disease model brains.

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Using hybrid molecular dynamics-lattice Boltzmann simulations to study polymers and porous particles in confined environments

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We present a numerical study of the dynamics of solid and porous microparticles and polymers in channels and T-shaped junctions. Good agreement with experimental data is obtained on the location of particle-separating streamlines for single solid particles with realistic parameters corresponding to the experiments. We quantify the changes in the position of the separating line for porous, partially penetrable colloids. A prediction of the full phase diagram for particle separation is presented in the case of two successive particles entering a T-junction. We also consider the statics and dynamics of a flexible polymer confined between parallel plates both in the presence and absence of hydrodynamic interactions. We consider two cases: (i) confinement for both the solvent and the polymer, and (ii) confinement for the polymer only (in a 3D solvent), which is experimentally feasible, for instance, by (optical) trapping. We find a continuous transition from 2D to 3D dynamic scaling as a function of decreasing degree of confinement within the de Gennes and the weak-confinement regimes. We demonstrate that, in the presence of hydrodynamics, the polymer's center-of-mass diffusion coefficient in the direction parallel to the walls scales differently as a function of the level of confinement in cases (i) and (ii).

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Interactions of extended peptide conformations and β-sheet formation

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In this presentation, we will discuss interactions of extended conformations of homodimeric peptides made of small (glycine or alanine) and large hydrophobic (valine or leucine) sidechains using all-atom computer simulations to decipher driving forces behind β-sheet formation. Dimers adopt β-sheet conformations at short inter-peptide distances ($\xi \sim 0.5$ nm) while at intermediate distances (~ 0.8 nm), dimers made of valine or leucine assume "cross-β like" conformations with sidechains interpenetrating each other. These two states are identified as minima in the Potential of Mean Force (PMF). While the number of inter-peptide hydrogen bonds increases with decreasing inter-peptide distance, the total hydrogen bond number in the system does not change significantly, suggesting that formation of β-sheet structures from extended conformations is not driven by hydrogen bonds. This is confirmed by an increase in electrostatic energy at short inter-peptide distances. A remarkable correlation between the volume of the system and the total electrostatic energy is observed, supporting the view that excluded water regions in proteins have an enthalpic penalty. We will also discuss microscopic mechanisms accounting for β-sheet formation based on computed enthalpy and entropy and we will show that they are different for peptides with small and large sidechains.

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Investigating Peptide/RNA Binding Using Enhanced-Sampling Simulation Techniques

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Studying peptide/RNA binding is of great biological and pharmaceutical importance. However, computer-aided drug-design targeting RNA faces several difficulties including the RNA flexibility [2] and the highly charged nature of RNA molecules [3]. Promising prospects are coming from the development of more accurate force fields for RNA [4, 5] and enhanced sampling methods [6, 7, 8, 9], which allow better and faster ways of investigating ligand/RNA complex formation.

We here present a computational protocol which allows studying the binding of RNA molecules and charged peptides using atomistic, explicit-solvent molecular dynamics simulations coupled with enhanced-sampling techniques. In our method, a suitable estimate of the electrostatic interaction is used as a reaction coordinate (collective variable) which is then accelerated using bidirectional steered molecular dynamics [6, 8] and well-tempered metadynamics simulations [7, 9]. Since the electrostatic interaction is only used as a collective variable to enhance the sampling, the approximations employed to compute it do not affect the final accuracy of free energy calculations. The method is applied to characterize the binding of TAR RNA from HIV-1 and a small cyclic peptide. Our simulation protocol allows blindly predicting the binding pocket as well as the binding affinity. Such a self-guiding feature is important since it is applicable even when experimental information in unavailable, which is the case of most computational drug designs. The method is general and not limited to peptide/RNA bindings, thus could be applied to study other electrostatics-driven binding events.

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Phase Field Crystal Modelling of Magneto-Elastic Effects in Isotropic Ferromagnetic Solids

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Magnetic hardness (coercivity) is an important property of ferromagnetic materials that characterized their hysteresis curve and their applications. Being an essential component of many electronic devices, magnetic materials are at the root of progress in electrical engineering and electronics and material science.

In this work we studied the inter-relation between morphological structure and magnetic properties, specifically the dependence of coercivity on the grain size in isotropic ferromagnetic solids. We constructed a minimal free energy functional (Magnetic PFC model) to incorporate elastic and magnetic properties of isotropic ferromagnetic solids. The free energy is an extension of the phase-field crystal free energy functional [1] with additional terms to include the paramagnetic to ferromagnetic phase transition and magnetostriction effects. The phase diagram of the model was calculated. The equilibrium phases include liquid, ferromagnetic hexagonal solid and non-magnetic solid phases. Using amplitude expansion method, we calculated the free energy in terms of the strain tensor elements which allowed us to study the magnetostriction effect, hysteresis properties and the effect of the grain boundary on coercivity. In particular we derived a relation for the dependence of coercivity on the grain mis-orientation angle in the isotropic limit.

Numerical simulations were performed to further study the properties of the model. The relation between the grain size and the coercive force was analyzed and we found a qualitative agreement with the experiments on soft magnetic nanocrystalline materials as reported in [2].

The Magnetic PFC model which was constructed in this research, has essential properties that make it ideal to study magneto-elastic effects in ferromagnetic materials or (with a minor change) for electro-elastic effects in piezoelectric materials. Even though in this model the free energy is written in terms of the coarse-grained order parameters, it still resolves the atomic scales and therefore many properties that originate from microscopic scales, such as elastic and plastic properties, defects and grains are included in this model. The model also averages the order parameters over time, which allows simulations to reach time scales that are necessary to observe the phenomena that happens in diffusive time scales such as diffusion of defects, grain growth and formation of microstructures. These are the distinguishing properties in this model which are not achievable with other models used to study magneto-elastic effects.

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Velocity and energy distributions in microcanonical ensembles of hard spheres

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In a microcanonical ensemble (constant NVE, hard reflecting walls) and in a molecular dynamics ensemble (constant $NVE\mathbf{PG}$, periodic boundary conditions) with a number N of smooth elastic hard spheres in a d-dimensional volume V having a total energy E, a total momentum $\mathbf{P}$, and an overall center of mass position $\mathbf{G}$, the individual velocity components, velocity moduli, and energies follow transformed beta distributions with different arguments and shape parameters depending on d, N, E, the boundary conditions, and possible symmetries in the initial conditions. This can be shown marginalizing the joint distribution of individual energies, which is a symmetric Dirichlet distribution. In the thermodynamic limit the beta distributions converge to gamma distributions with different arguments and shape or scale parameters, corresponding respectively to the Gaussian, i.e., Maxwell-Boltzmann, Maxwell, and Boltzmann or Boltzmann-Gibbs distribution. These analytical results are in agreement with molecular dynamics and Monte Carlo simulations with different numbers of hard disks or spheres and hard reflecting walls or periodic boundary conditions.

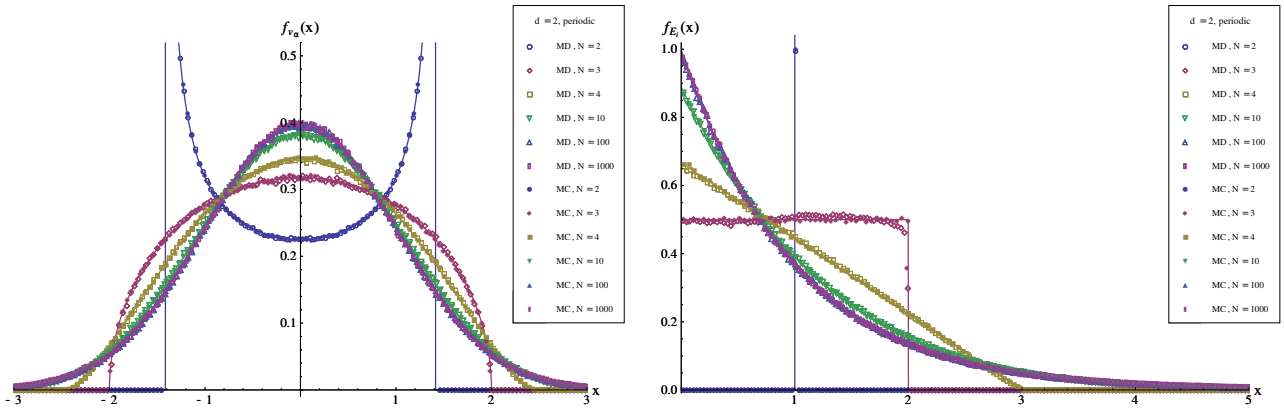

Figure 1: Probability density functions $f_{v_{i\alpha}}$ of the velocity components (left) and f_{E_i} of the energy (right) for $N = 2, 3, 4, 10, 100, 1000$ hard disks with $\bar{E} = 1$ in a two-dimensional ($d = 2$) molecular dynamics ensemble: theory (lines), MD (empty symbols), and MC (full symbols).

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Nonequilibrium Methods for Calculating the Potential of Mean Force for Biomolecular Systems

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The potential of mean force (PMF) serves as an effective potential and is a key quantity used to calculate interactions in peptide, protein, and membrane systems. Our group has developed some new and practical nonequilibrium work methods of calculating the PMF, based on the theorems of Jarzynski, Crooks and Kosztin. Applications to be described include calculations of the binding free energies of peptide-peptide and peptide-membrane systems. The methods used to calculate the PMF yield simultaneously the local diffusion coefficient of the molecules involved, and thus, from the PMF and the local diffusion coefficient, enable one to calculate the permeability coefficient using the theory of Marrink and Berendsen. Calculations of membrane permeability coefficients for molecules and ions will be discussed.

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Intrachain ordering and segregation of polymers in a confined space

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Cylindrical confinement can induce linear ordering in individual polymer chains and enhance their segregation tendency similarly to what is observed for bacterial chromosomes. I will discuss the relationship between intrachain ordering and segregation of two polymers confined in a cylindrical space, and show that the *E. coli* chromosome is in the linear-ordering and spontaneous-segregation regime.

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Flow of spherical micellar solutions in confined channels

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We use molecular-dynamics simulations to study the structural and dynamical properties of a coarse grained (CG) model of surfactants in micellar solution under flow in a die-extruder geometry. Variations in flow and surface-surfactant interactions lead to rich behavior including fragmentation and re-assembly of micelles. We examine the effect of flow, confinement, and wetting on spherical micelles. We use sodium dodecyl sulfate (SDS) as our model system which has been extensively studied, both experimentally and computationally. Our previous atomistic MD simulations of SDS system under varying conditions [1, 2] provide a good reference system for this study.

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Dynamics of water molecules: Rockin' and jumping

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Hydrophobic hydration has been debated intensly since the seminal paper by Frank and Evans in 1945 [1]. The "iceberg" model has been probed by experiments and simulations with controversial results. In this talk we will discuss hydrophobic hydration and the iceberg model based on our results from >100 ps *ab initio* simulations [2]. We discuss the relation to femtosecond spectroscopy measurements and the consequences to proteins and other systems. It will be demonstrated that water dynamics cannot be described by simple Debye rotational diffusion but instead, water molecules execute large angle jumps.

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Stability and Cooperativity of Protein Folding in Crowded and Confined Environments

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In living cells, the presence of biomacromolecular crowders strongly affects the stability of folded proteins. The overall effects depend on the size and concentration of the crowding agents as well as on its chemical properties. In a recent publication [1] we employ a simple Go model of the Trp-cage protein in spherical solvents to assess the effects of macromolecular effects on protein stability. The computer simulation model uses a single control parameter ε_{ps} that varies the protein affinity of the spherical solvents. Repulsive solvents, $\varepsilon_{ps} > 0$, which mimics protein-protecting osmolytes, stabilize the structure of folded proteins, increasing the folding temperature. Attractive solvents, $\varepsilon_{ps} < 0$, mimics denaturants (such as urea), destabilizes proteins, decreasing the folding temperature. Data analysis that used the weight histogram method (WHAM) found an entropy-driven stabilization mechanism of proteins by osmolytes. In contrast, denaturants destabilize proteins by an enthalpy-driven mechanism. The model was generalized to include variation in solvent size and volume fraction [2], as well as to protein in confinements. The confined proteins are encapsulated in hydrophobic or hydrophilic rectangular walls, to mimic the chaperonin GroEL/ES. The cooperativity of the systems are assessed by the method developed by Chan and coworkers [3]. In general, the cooperativity remains the same for confined proteins and proteins in denaturants, but in some cases, the cooperativity decreases in the presence of osmolytes, despite an increase in the stability of the native state. This unusual behavior is attributed to the loss of conformation entropy due to osmolytes.

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Colloidal Particles Interacting in a Cholesteric Liquid Crystal

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Using a lattice-Boltzmann algorithm, we investigate the interactions among colloidal particles immersed in a cholesteric liquid crystal. These interactions arise due to a preferred orientation of the liquid crystal molecules on the colloidal surface, leading to the formation of defects and distortions in the bulk liquid crystal. If tangential anchoring is preferred at the colloidal surface, the two point defects, present at the poles of a particle in a nematic, each split into a pair of defects connected by a 1/2 defect line winding around the particle in the bulk liquid crystal. If instead perpendicular anchoring is assumed at the particle surface, the usual Saturn ring defect, present in a nematic, becomes twisted around the particle. When more than one particle is present, defect lines associated with nearby particles tend to join together in order to minimize the system energy. Here, we present results for chains and a diamond structure, produced as a result of these interactions.

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Multiple Replica Repulsion Technique for Efficient Conformational Sampling of Biological Systems

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We propose a technique for sampling complex molecular systems with many degrees of freedom. The technique, termed "multiple replica repulsion" (MRR), does not suffer from poor scaling with the number of degrees of freedom associated with common replica exchange procedures and does not require sampling at high temperatures. The algorithm involves creation of multiple copies (replicas) of the system, which interact with one another through a repulsive potential that can be applied to the system as a whole or to portions of it. The proposed scheme prevents oversampling of the most populated states and provides accurate descriptions of conformational perturbations typically associated with sampling ground-state energy wells. The performance of MRR is illustrated for three systems of increasing complexity. A two-dimensional toy potential surface is used to probe the sampling efficiency as a function of key parameters of the procedure. MRR simulations of the Met-enkephalin pentapeptide, and the 76-residue protein ubiquitin, performed in presence of explicit water molecules and totaling 32 ns each, investigate the ability of MRR to characterize the conformational landscape of the peptide, and the protein native basin, respectively. Results obtained for the enkephalin peptide reflect more closely the extensive conformational flexibility of this peptide than previously reported simulations. Those obtained for ubiquitin show that conformational ensembles sampled by MRR largely encompass structural fluctuations relevant to biological recognition, which occur on the microsecond timescale, or are observed in crystal structures of ubiquitin complexes with other proteins. MRR thus emerges as a very promising simple and versatile technique for modeling the structural plasticity of complex biological systems.

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Role of dipolar interactions in protein folding

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A generic coarse-grained (CG) protein model is presented with two beads per amino acid (backbone and side-chain) with explicit solvation. The side-chain is modeled using four different bead types: hydrophobic (H), polar (P), positively or negatively charged whereas the backbone is modeled with a polar bead. The solvent is modeled using the polarizable MARTINI water model[1]. The change in orientation of the atoms in the coarse-grained unit is captured by the addition of Drude oscillators[2,3] inside each polar coarse-grained bead. The addition of dummy sites inside the polar beads introduces structural polarization into the coarse-grained model.

Realistic α/β content is achieved *de novo* without any biases in the force-field toward a particular secondary structure. The dipoles created by the Drude oscillators interact with each other and drive the protein models to fold into unique structures depending on the amino acid patterning and presence of capping residues. In this talk, we will show the role of dipole-dipole and dipole-charge interactions in shaping the secondary and tertiary structure of proteins. In particular, we will focus on the folding of β-hairpins and single helices (see Figure 1) and in helix bundles and multiple β-sheet strands. In the folded ensemble, dipoles along a helix are found aligned parallel and stabilized by the presence of charged capping residues. On the other hand, β-sheets exhibits antiparallel neighbouring dipoles.

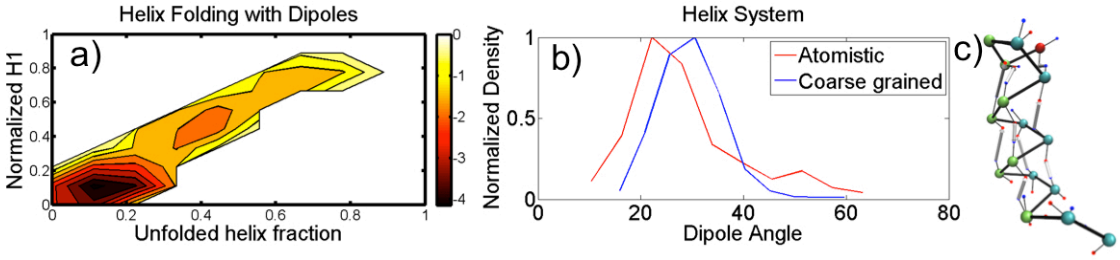

Figure 4: a) Free energy profile as a function of the unfolded helix fraction and normalized H1 (between *i* and *i*+3 backbone beads) distance. b) Comparison of dipole angles between the dipoles created in the folded helical conformation of the coarse-grained model by the dummies and the dipoles created by the atoms N-H of amino acid *i* and atom O of amino acids *i*+4 in a polyalanine helix with all-atom resolution. c) Most populated conformation of the folded ensemble. Only backbone beads are shown. Cyan beads correspond to hydrophobic beads, green to polar and red to a positive charge bead. Dummy particles are shown in a smaller size. Dipoles are shown by arrows.

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A Numerical Study on Tissue Topology Using Single Cell Based Model

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Tissue topology, such as proliferating epithelium topology, shows striking similarities for various species. This suggests unified mechanism for tissue formation which can be explored with the help of physical or mathematical models. Indeed, it has been shown that cell divisions along with local cell rearrangements can reproduce commonly observed epithelium topology by using topological models[1].

Tightly packed cells in epithelium resemble polygons. This observation gave rise to models where cells are treated as polygons in junctional network[2]. These models were used to investigate effects of cell mechanics and cell divisions on topology.

In some cases cells undergo extensive rearrangements during tissue formation which dramatically alters tissue topology. Based on our previous work[3], we propose single cell based mechanical model which can naturally account for cell rearrangements. Importantly, this model takes into account cell elasticity and adhesion. Cell growth is controlled by hydrostatic pressure.

In this work, we study the influence of cell mechanics and various division mechanisms on tissue formation. We also consider different growth mechanisms and investigate their effects on tissue topology.

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Various approaches for accelerating sampling of protein conformation : from amyloids to loop motion

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Sampling protein conformations remains a significant challenge in spite of considerable growth in available computational resources and numerous approaches have been proposed to address this issue. Over the last years, we have used a number of approaches for increasing sampling, including activated and multiscale methods, such as the activation-relaxation technique (ART nouveau), for searching through the conformational space and the use of various coarse-grained models. I will present here applications of these approaches to protein aggregation, protein folding and loop flexibility, focusing on examples of applications on protein A, amyloid aggregation, polyglutamin, calmodulin and troponin C. I will also discuss a new coarse-grained potential that we are currently developing.

This work is done in collaboration with Sébastien Côté, Lilianne Dupuis, Cindie Eugène and Jean-François St-Pierre at Université de Montréal as well as Philippe Derreumaux (IBPC, France) and Pierre Tuffery (Université de Paris 7). It is supported by the Canada Research Chair Foundation,the FRSQ and NSERC. Computer resources are generously allocated by Calcul Québec/Compute Canada.

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Understanding beta-sheet stabilization – lessons from a model hairpin peptide

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Proteins fold into specific conformations, dictated by their primary sequence, resulting in unique functions. Protein misfolding is associated with the failure of proteins to adopt native state structures. A variety of human diseases including Alzheimers', Parkinson's and type II diabetes are associated with incorrect protein folding [1]. Conversion of loop or helical regions of proteins to beta-sheet conformations that self-assemble into fibrils is observed in several misfolding diseases [2,3]. Determining factors contributing to stability of beta-sheets are crucial to understanding the conformational transitions leading to misfolding diseases. Beta-hairpin peptides form basic components of anti-parallel beta-sheets and are suitable model systems for characterizing the fundamental forces stabilizing beta-sheets implicated in disease states. In this study, we use the 16-residue C-terminal fragment of protein GB1 to understand the structural and thermodynamic components stabilizing the beta-hairpin conformation. We have performed molecular dynamics simulations of GB1 peptide in explicit water at 298 K using the GROMACS software package [4]. The free-energy landscape is determined from the potential of mean force. We show relationships between the different energetic terms and the free energy minima corresponding to beta-hairpin conformations. Our analysis sheds light on energetic components to stabilize beta-hairpin conformations, which can be extended to explain the stability of beta-sheets in disease states.

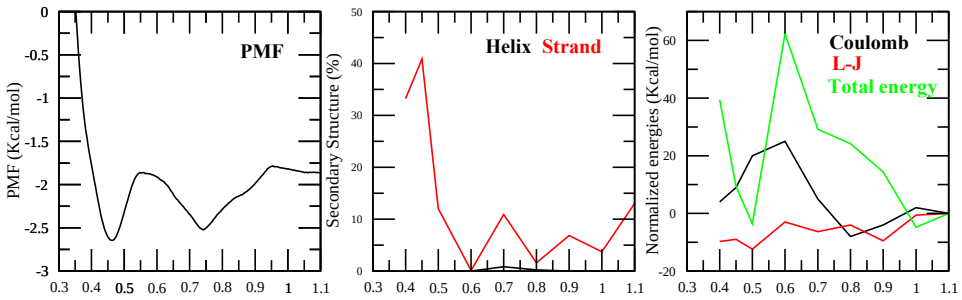

Figure 1: a) Potential of mean force, b) secondary structure and c) normalized values for the total, electrostatic and Lennard-Jones energies as a function of the end-to-end distance .

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Computational Studies of Peptide and Proteins in Lipid Membranes

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Many interesting biological and biophysical processes involve interactions between peptides or proteins and lipid or detergent molecules. The detailed characterization of these processes is currently impeded by the difficulty to elucidate the structure of peptides and proteins in the anisotropic and chemically complex environment provided by lipid bilayers and detergent micelles. We use atomistic computer simulation techniques to examine the structural and physical basis for these interactions in studies combining efficient sampling algorithms with massive computing. I will describe how lipid and detergent self-assemblies solvate proteins and determine their fold; and reciprocally, how the insertion and self-aggregation of toxic peptides affect the structure of lipid bilayers.

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Frontiers in Membrane Biophysics

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One of the major challenges of modern physics is to contribute to biology and life-sciences. Neutron and X-ray beams enable us to study molecular structure and dynamics in membranes in-situ, under physiological conditions [1].

The experiments give access to nanoscale to mesoscopic diffusion processes, effects of macromolecules, such as ethanol and cholesterol on membrane properties, the interaction with drugs, such as aspirin and ibuprofen, detection of raft structures and protein-protein interactions between trans-membrane proteins. I will talk about current topics in membrane biophysics and the associated experimental challenges and present exciting recent results and potential biomedical applications. Our quantitative results lend themselves for comparison with computer simulations of complex membrane systems.

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Escape from adaptive conflicts in the evolution of protein folds: bi-stability, mutational robustness, and gene duplication

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Proteins are long heteropolymeric chain molecules that form (fold into) distinct, compact three-dimensional structures. This structure determines a protein's biochemical function within a cell. Many organisms live under complex and changing environmental conditions, while having a limited number of proteins to deal with these conditions. Multi-functionality, as exhibited by many functionally promiscuous enzymes, has been hypothesised as an advantageous compromise whenever the same protein is under Darwinian selection to conserve an existing function while also adapting towards (or being co-opted for) a new function, a situation referred to as 'adaptive conflict'. A stage of multi-functionality may or may not be followed by gene duplication and divergence [3, 2]. We use a simple biophysical model [1] to explain the basic principles behind the multi-functionality of proteins that can fold into more than one stable structure (using structure formation as a proxy for functionality). Using a statistical mechanics description of all possible structural states, and due to the coarse grainedness of the model, it is possible to keep track of non-ground state structures and to identify degenerate ("multi-functional") ground states. Our model predicts that proteins evolving under selection for two alternative structures can follow gradients of stability shift from the formation of only one stable structure towards an equilibrium state between two stable structures (bi-stability), each providing an independent function [4]. Population dynamics simulations show that weak conflicting selection pressures may be sufficient to direct protein evolution towards bi-stability. Our results also suggest that models of protein evolution may underestimate evolvability if they do not account for bi-stability. However, while bi-stable proteins provide many more mutational connections to other protein structure phenotypes in genotype space, they are also less stable. This shows the inherent conflict between conservation of structure (by maximising stability), and adaptation towards new structures (which requires some destabilisation). Bi-stable proteins may provide the necessary compromise. Furthermore, bi-stable proteins may provide an additional advantage after gene duplication, because they provide excellent starting points for subfunctionalisation (functional divergence driven by adaptation and/or genotype space entropy), as consistent with the 'Escape from Adaptive Conflict' model [5]. The potential for increased evolvability due to bi-stable proteins is thus two-fold by allowing adaptation before and after gene duplication.

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Exploring the Polyelectrostatic Model of Sic1-Cdc4 Interaction using Coarse-Grained Explicit-Chain Simulations

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Intrinsically disordered proteins (IDPs) or protein regions often serve crucial functions in biological signaling and regulation, wherein phosphorylation of the IDP is a common means of modulating the pertinent protein-protein interactions. DNA replication in yeast can only be initiated after eliminating the cyclin-dependent kinase inhibitor Sic1 via the SCFcdc4 ubiquitin ligase; but the binding between Sic1 and substrate adapter subunit Cdc4 can only occur after phosphorylation of a minimum of around six of the nine cyclin-dependent kinase sites on Sic1 [1]. To account for this ultrasensitive behavior, a mean-field statistical mechanical model was developed. The model posits that the negative charges on the multiple Sic1 phosphorylation sites contribute to binding stability even though they are not in direct contact with the positively charged binding pocket which consists of four Arginine residues. This mode of interaction, term "polyelectrostatic," is consistent with existing experimental data [2]. To further assess the validity of the polyelectrostatic hypothesis, we have now developed a coarse-grained explicit-chain model for the Sic1-Cdc4 interactions using a Poisson-Boltzmann treatment of electrostatics. Predictions from our explicit-chain simulations are in general agreement with the earlier mean-field model, underscoring once again that polyelectrostatic interactions may provide a powerful general framework for understanding IDP interactions that involve multiple phosphorylation sites. The present chain model also provides additional information such as the distribution of residence time among different phosphorylation sites in the single binding pocket, which is in general agreement with experiment [3]. These new predictions are amenable to future experimental testing.

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MARTINI coarse-grained and atomistic simulations of lipids

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Computer simulations have been widely used to study properties of lipid aggregates. Over the past twenty years simulations have progressed from small models of lipid bilayers composed of one type of lipid at length scales of 5-8 nanometer and time scales of nanoseconds to very complex models at length scales of tens of nanometers and time scales of microseconds. The development of realistic coarse-grained models such as the MARTINI model [1,2] has brought simulations of lipids to mesoscope scales where particle-based simulation and continuum models overlap and simulations can be compared to measurable mechanical parameters of lipid aggregates. MARTINI is parameterized primarily based on experimental data, but for many systems of biological importance there is limited experimental data that can be used in parameterization and validation. I will discuss recent progress in linking atomistic simulations, experimental results, and parameters from continuum models to MARTINI simulations, illustrated with examples on lipid mixtures [3], membrane tethers [4], and lipid-protein systems.

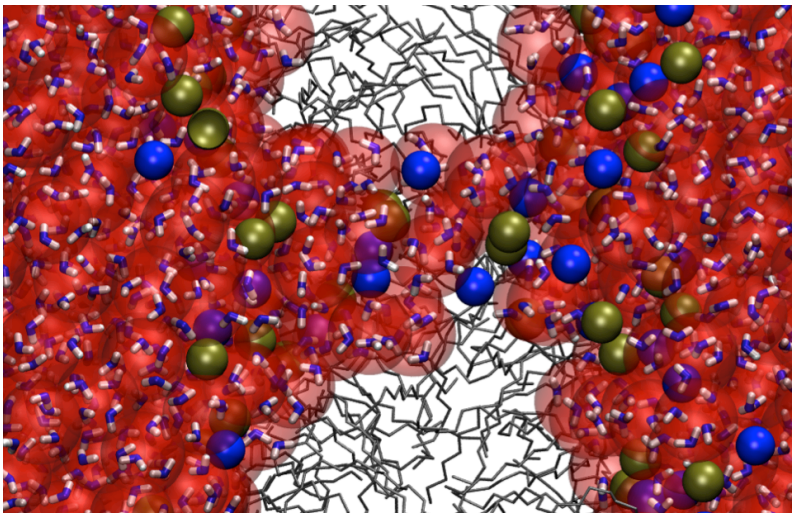

Figure 1: Water-filled pore in a membrane model, with both atomistic and coarse-grained representations.

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Ordered Mononucleotide Arrays in Multi-lamellar Lipid Matrices: Implications for the Origin of Life

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How nucleic acids first assembled and were then incorporated into the earliest forms of cellular life 4 billion years ago remains a fundamental question of biology. It is postulated that prior to today's DNA, RNA, and protein dominated world, RNA (ribonucleic acid) was used as genetic storage and a catalyst to chemical reactions.

RNA is a polymer chain of nucleotides bound together forming a ribose-phosphate backbone. The polymerization of nucleotides occurs in a condensation reaction in which phosphodiester bonds are formed. In this study, we used X-ray scattering to investigate 5'-adenosine monophosphate (AMP) molecules captured in a multilamellar phospholipid matrix composed of dimyristoylphosphatidylcholine (DMPC) Ref. [1], as shown in Fig. 1.

We observe evidence of lateral organization of the confined mononucleotides: instead of forming its natural crystal structure or geometrically favourable herringbone or chevron structures, the AMP molecules are highly entangled. This structure requires energy to form, which is thought to be provided by the lipid bilayer. The close proximity of the phosphate and ribose groups in this structure may facilitate condensation reactions that link these molecules into a nucleic acid strand. A more complex mixture confined by a lipid bilayer to find the structure of binding pairs in a lipid matrix will be the next step in the investigation of the synthesis of RNA.

This experiment is the first demonstration that lipids can in fact organize potential monomers within a matrix and thereby promote polymerization into RNA-like polymers.

This system lends itself to comparison with computer simulations for the investigation into physical mechanisms behind RNA formation under early earth conditions.

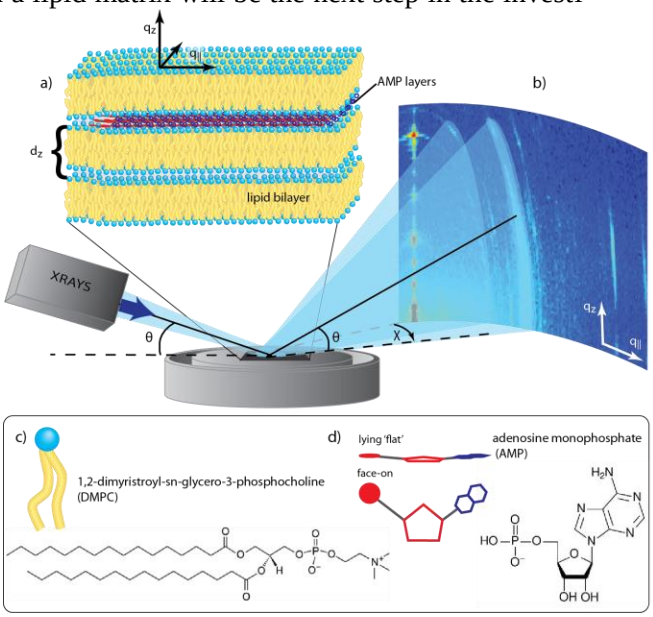

Figure 1: Schematic of the X-ray diffraction experimental set-up. a) Highly oriented lipid bilayers containing AMP layers.b) Two-dimensional X-ray diffraction data. C) The lipid used: DMPC. d) Nucleotide used: AMP.

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Calculating Free Energy of the Aggregation of the Peptide (HHC-36) In Bulk

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The increasing demand for antibiotics has contributed to the investigation of possible novel antibiotics by many researchers. For this purpose, experimental and theoretical studies have been carried out to draw scientists' attention to antimicrobial peptides and their interaction with the surface of bacterial membranes. Their ability to disrupt the functioning of bacterial membranes has been probed from different perspectives. The most desirable antimicrobial peptides are those which do not harm plant or animals' membranes but which disrupt bacterial membranes. It has been found that some cationic antimicrobial peptides (CAPs) satisfy these requirements. CAPs interacting with the outer membrane of gram-negative bacteria and the membrane of grampositive bacteria have been studied recently.

We conduct a Molecular Dynamics simulation study of peptide-peptide interactions inphysiological solutions and investigate the mechanism of CAPs aggregation, since aggregation of the peptides could precede their interaction with the membrane. Different algorithms are applied to calculate the potential mean force of the aggregation process of peptides to select the most efficient one. Also, we have run CD spectroscopy and calorimetry experiments to predict the structure of the peptide and measure the peptide-peptide binding enthalpy, and compared these results with our simulation data. The particular CAP studied is HHC-36, a peptide selected by high throughput screening [1-3] which has nine amino acid residues and charge +5.

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Variational Problems of Physical Origin (SS-VPPO)

Organizers:
Robert Jerrard (University of Toronto)
Andrew Lorent (University of Cincinnati)

This minisymposium will be devoted to rigorous mathematical results on problems from the calculus of variations that are motivated by applications to physical models. Physical problems that will be considered are likely to include descriptions of vortices in superconductors and superfluids, as modelled by the Ginzburg-Landau and Gross-Pitaevskii functionals respectively; problems related to nonlinear elasticity, including rigidity in multiwell elasticity and the elastic behaviour of thin films; and behaviour of diblock copolymers and related variational models involving nonlocal perturbations of the perimeter functional.

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STABLE VORTEX STATES IN SUPERCONDUCTIVITY

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We present the construction of local minimizers to the Ginzburg-Landau functional of superconductivity. In the presence of an external magnetic field of large enough strength, a superconductor responds to it by creating topological defects known as vortices where the field penetrates the sample. We investigate the existence of stable states where the number of vortices is far from optimal(as dictated by the energy formulation). We review some of the history behind the problem(cf. [**?**]) and conclude by exhibiting local minimizers whose number of vortices N is prescribed and blows up as the parameter epsilon, inverse of the Ginzburg-Landau parameter kappa, tends to zero. We treat the case of N as large as log epsilon, and a wide range of intensity of external magnetic field. The vortices of our solutions arrange themselves with uniform density over a subregion of the domain bounded by a "free boundary" determined via an obstacle problem, and asymptotically tend to minimize the "Coulombian renormalized energy" W introduced by Sandier and Serfaty. This is joint work with Sylvia Serfaty(cf. [**?**]).

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Front speed enhancement by large incompressible flows in 3 dimensions

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We consider a scalar reaction-advection-diffusion equation

$$u_t = \nabla \cdot (A(x)\nabla u) + M\, q(x) \cdot \nabla u + f(x,u), \quad t \in \mathbb{R},\ x \in \mathbb{R}^N. \tag{1}$$

with a KPP nonlinearity in a heterogeneous periodic setting. A typical homogeneous KPP nonlinearity $f(u) = u(1-u)$. Heterogeneity appears in (1) through the dependence of the coefficients on the space variables as well as the presence of a large advective term $Mq \cdot \nabla u$ where q is an incompressible field and M is understood as a large parameter. A special feature of (1) is that it admits traveling-waves-like solutions: fixing a direction $e \in \mathbb{R}^N$, one seeks particular solutions of (1) which are of the form $u(t,x) = \phi(x \cdot e - ct, x)$ which connect the stationary states 1 and 0 by $\phi(-\infty, x) = 1$ and $\phi(+\infty, x) = 0$, uniformly in x. Biological invasions are indeed one of the most common examples of propagation phenomena and (1) seems to be the most widely used equation in ecological and biological modeling. In the homogeneous setting (the diffusion A and the reaction f in (1) do not depend on x and the advection $q \equiv 0$), there exists a spectrum of speeds $[c^* = 2\sqrt{f'(0)}, +\infty)$ such that a traveling front (c,u) exists if and only if $c \geq c^* = 2\sqrt{f'(0)}$. In a heterogeneous setting, an analogous result is well known nowadays (thanks to several works by H. Weinberger (2002), Berestycki-Hamel (2002), J. Xin (2000) and many others): there exists a minimal speed $c^* = c^*_{A,q,f}(e)$. However, the value of the this minimal speed was given via a *variational formula involving elliptic eigenvalue problems* in [2]. The minimal speed $c^*_{A,q,f}(e)$ is the most interesting among all others in the interval $[c^*, +\infty)$ as it describes the spreading of initial data for the related Cauchy problem. The presence of an advection in (1) is expected to enhance the propagation (think of stirring for instance). Indeed, it was proved in [1] that the quantity $(c^*_{Mq})/M$ remains bounded independently of M. In [3], we gave the precise $\lim_{M\to+\infty} c^*_{Mq}/M$ in a *variational form* which involves "*first integrals*" of the incompressible flow q. These are H^1_{loc} functions w which satisfy $q \cdot \nabla w = 0$ a.e. We also gave a sharp criterion, in the case $N = 2$, on the flow q so that the limit of $\frac{1}{M} c^*_{Mq}$ is positive. Our results in [3], together with those in [5, 6], led to clear understanding of the asymptotic regimes of the minimal speed within large drift, in the 2 dimensional case. The goal of this talk is to show recent results in the 3 dimensional case. We establish a link between ergodicity and first integrals. This link will allow us to find a class of flows which are not shear flows, admit an ergodic nature and linearly speed-up the KPP fronts.

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Variational problems with nonlocal operators

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We study the nonlocal and nonlinear problem

$$\begin{aligned} L\phi + V\phi - |\phi|^2 * W\phi &= -\lambda\phi, \\ \|\phi\|_{L^2(R^3)} &= 1, \end{aligned}$$

for a large class of potentials V and W. The operator $L = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2}$ (the quasirelativistic Laplacian), with α being Sommerfeld's fine structure constant, is a nonlocal, pseudo differential operator of order one. We prove the existence of multiple solutions for two separate cases: (1) unconstrained problem; (2) constrained problem. Similar problems and results are presented for the case when a convection term is included; the problems arise in plasma theory (Hartree-Fock type models).

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Thin limit theories in nonlinear elasticity and infinitesimal isometries

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We will describe how the rigorous study of a generic nonlinear thin elastic shell from a variational point of view gives rise to some important questions regarding the behavior of the Sobolev-type infinitesimal isometries on the mid-surface of the shell. Questions of interest include the rigidity, regularity, approximation by smooth isometries and matching to higher order isometries [1, 2, 3, 4]. In the latter context we will discuss a recent result which states the following: Assume that $\Omega \subset \mathbb{R}^2$ is a simply-connected domain and that $v, v_0 \in C^{2,\alpha}(\Omega)$ are such that

$$\det\nabla^2 v = \det\nabla^2 v_0 \geq c \text{ in } \Omega,$$

for some $c > 0$. Then there exists an equibounded family of mappings $w_\varepsilon \in C^{2,\alpha}(\Omega, \mathbb{R}^3)$ such that for all $\varepsilon > 0$,

$$\nabla(\mathrm{id} + \varepsilon v e_3 + \varepsilon^2 w_\varepsilon)^T \nabla(\mathrm{id} + \varepsilon v e_3 + \varepsilon^2 w_\varepsilon) = \nabla(\mathrm{id} + \varepsilon v_0 e_3)^T \nabla(\mathrm{id} + \varepsilon v_0 e_3),$$

where $e_3 = (0,0,1)$ and $\mathrm{id} : \Omega \to \mathbb{R}^3$ is given by $\mathrm{id}(x,y) := (x,y,0)$.

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Women in Science and Mathematics (SS-WSM)

Organizers:
Shohini Ghose (Wilfrid Laurier University)
Hind Al-Abadleh (Wilfrid Laurier University)

Women have made important contributions to science, mathematics and computer science. The first computer algorithm was written by Ada Lovelace, daughter of the poet Lord Byron. This session will highlight research in applied mathematics, modeling and computational science by female researchers. It will also include talks and a panel discussion about gender issues in mathematics and science.

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Zero–Hopf bifurcation in the hyperchaotic Lorenz system

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We characterize the zero-Hopf bifurcation at the singular points of the next hyperchaotic Lorenz system:

$$\begin{aligned} \dot{x} &= a(y-x)+w, \\ \dot{y} &= cx-y-xz, \\ \dot{z} &= -bz+xy, \\ \dot{w} &= dw-xz. \end{aligned} \tag{1}$$

We can find in the literature several so called hyperchaotic Lorenz systems, see for instance [2, 3, 4, 5]. We remark that not all of these hyperchaotic Lorenz systems coincide, they can vary in one or more therms. The system (1) has been studied in [3, 5].

The method developed for studying the zero-Hopf bifurcation of this hyperchaotic Lorenz systems is based on averaging theory. This method can also be applied to other differential systems in $\mathbb{R}^n$.

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Topos Formulation of Quantum Theory

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As it stands, the mathematical formulation of quantum theory leads to a non realist interpretation of the theory. In particular, the mathematical way in which certain objects are defined, such as the state space, the concept of propositions and other, imply that prop- erties cannot be said to be possessed by quantities. All that can be said is that, if a measurement is performed a large amount of times, then a certain result will be obtained with a given probability. This is the so called relative frequency interpretation of quantum theory (or Copenhagen interpretation). However, the applicability of such an interpretation requires a sharp distinction between the notion of observer and observed system leading to the well known measurement problem. A possible way to overcome such a problem is by changing the mathematics with which to express quantum theory. This is the main idea behind the topos approach to quantum theory. In fact in this setting quantum theory is re-expressed in terms of topos theory instead of the standard mathematics of Sets. The resulting interpreta- tion is more realist in the sense that now it is possible to asses whether any set of quantum propositions, even incompatible ones, are true or false. The only caveat is that the notions of true and false are not the classical notions. In fact we end up with a multivalued, intuitionistic type logic. However, such a logic allows for a representation of proba- bilities in terms of truth values. Thus, in this setting, probabilities are given a logical interpretation which enables to overcome the relative frequency interpretation of probabilities.

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The Power of Diversity:Women's Leadership in STEM

Judith C. Giordan

ecosVC, Inc and The Chemical Angels Network

The case for diversity in leadership is the case for better organizations, better decisions and better actions. It is the case for improving reputation and organizational performance. It is the case for diverse approaches and opinions being collectively more effective than that of any one "expert" or traditionally accepted group of experts. It's in the math and in the data. And it is NOT only about women!

Yet women seem to be one of the most studied groups..and the numbers make a compelling case. Studies show that women can make the difference between economic success and failure in the developing world, between good and bad decision-making in the industrialized world, between profit and loss in the corporate world and between having and not having appropriate role models in higher science and engineering education. Conclusion: All organizations would do well with more women in leadership positions. [1]

And the contention is substantiated by data…

- Pepperdine University found that the Fortune 500 firms with the best records of putting women at the top were 18 to 69 percent more profitable than the median companies in their industries.
- McKinsey looked at the top-listed European companies and found that greater gender diversity in management led to higher-than-average stock performance.

And the results from the NSF funded study, Project ENHANCE[2], which studied over 1400 women formally trained in science, engineering and math and their managers provide statistically valid insights into the requirements of women and their management including that:

- Confidence is the single best predictor of career success for women.
- Women with greater opportunities for professional networking are more successful and satisfied with their jobs

With these data and concepts as a starting point, the presentation will explore options for women in science, math and engineering – and for the organizations in which they are employed – to increase value, organizational and personal reputation using the power of diversity *and* the power of women.

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Chemical Property Prediction based on Spectral Signature of Properties on Molecular Surfaces

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The great diversity of chemical structures lets us design materials with desired properties. This pursuit is hindered because finding the properties of all candidate molecules through experimental or computational studies is impractical. In many cases, performing proper experiments is time-consuming, expensive and unethical. Computational studies are also impossible in many cases; for example, it is impossible to compute properties related to macroscopic phenomena like physiological responses. These limitations can be overcome by adapting machine learning methods to the systematic, rapid and robust screening of large molecular datasets. This approach is feasible because of underlying smoothness in chemical property space: similar molecules have similar properties.

The main ingredients of molecular similarity modelling are a dataset of known molecules (the "training set"), an appropriate measure of molecular similarity and an estimation technique [1]. The traditional approach, three-dimensional quantitative structure-activity relationship (3D-QSAR), relates molecular structure to its chemical behavior; however, 3D-QSAR is limited by uncontrolled errors, difficulty in defining proper similarity measures and the need for significant insight from the practitioner. To overcome these obstacles, we exploit a machine-learning method called kriging that not only gives a prediction for the properties of unknown molecules, but also provides an estimate of the prediction error. We have combined kriging with the characteristic spectrum of property-values on the molecular surface. This encapsulates the key features of molecules and quantifies their similarity in universally-applicable, property-specific way. This approach is motivated by the recognition that chemical interactions are primarily determined by the properties of molecular surfaces and inspired by the way molecules are characterized using spectroscopy in experimental chemistry.

To demonstrate this technique, the protonation state of the nitrogen atoms in small, drug-like, organic molecules is predicted. We compute the electrostatic potential on a sphere centered on nitrogen atom as the molecule's reactivity descriptor and use the electrostatic-potential spectrum to predict the pK_a. The predicted pK_a of amines have small error, which is particularly promising given the simplicity of this first, proof-of-principle, test.

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Fast, recursive and numerically stable algorithms for discrete sine transformations having orthogonal factors

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Discrete Fourier Transforms (DFT) have numerous applications in sciences and engineering especially in applied mathematics and electrical engineering like signal processing, image processing, speech processing, feature extraction, convolution, solving partial differential equations and elsewhere, and they have been studied by authors, see, e.g., [1, 2, 3, 4]. There are real versions of the DFT called the Discrete Sine Transform (DST) and the Discrete Cosine Transform (DCT) of main variants I-IV.
Currently, there are no papers addressing the numerical stability of four main DST variants;

$$\begin{aligned} S^{I}_{n-1} &= \sqrt{\tfrac{2}{n}}\left(\sin\tfrac{(j+1)(k+1)\pi}{n}\right)_{j,k=0}^{n-2} \\ S^{II}_{n} &= \sqrt{\tfrac{2}{n}}\left(\varepsilon_n(j+1)\sin\tfrac{(j+1)(2k+1)\pi}{2n}\right)_{j,k=0}^{n-1} \\ S^{III}_{n} &= \left(S^{II}_{n}\right)^{T} \\ S^{IV}_{n} &= \sqrt{\tfrac{2}{n}}\left(\sin\tfrac{(2j+1)(2k+1)\pi}{4n}\right)_{j,k=0}^{n-1} \end{aligned} \tag{1}$$

where $\varepsilon_n(0)=\varepsilon_n(n)=\frac{\sqrt{2}}{2}$, $\varepsilon_n(j)=1$ for $j\in\{1,2,\cdots,n-1\}$ and n is an even integer. Moreover, the existing DST algorithms, though fast and recursive, are not based on orthogonal factors, and are unstable. This paper provides fast, numerically stable and recursive algorithms for four versions of the discrete sine transformation in terms of *sparse and orthogonal matrices*. Four new complete factorizations for discrete sine transformations are introduced, namely for DST I, DST II, DST III and DST IV. Also we were able to establish the *worst error bounds* of computing $y=Sx$ for each transformation $S^{I}_{n-1}, S^{II}_{n}, S^{III}_{n}$ and S^{IV}_{n}. By using the former result we were able to show that the algorithms for DST I-IV are *forward and backward stable*. Due the nature of the factorizations of each of the DST I-IV algorithms these are easy to implement and use only permutation matrices, orthogonal sparse matrices, rotation/rotation-reflection matrices and butterfly matrices and, produce numerically stable $O(n\log n)$ complexity algorithms.

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Fifteen Years of Funded Programs to Advance Women in Science and Engineering: Progress and Persistent Challenges

C. Mavriplis

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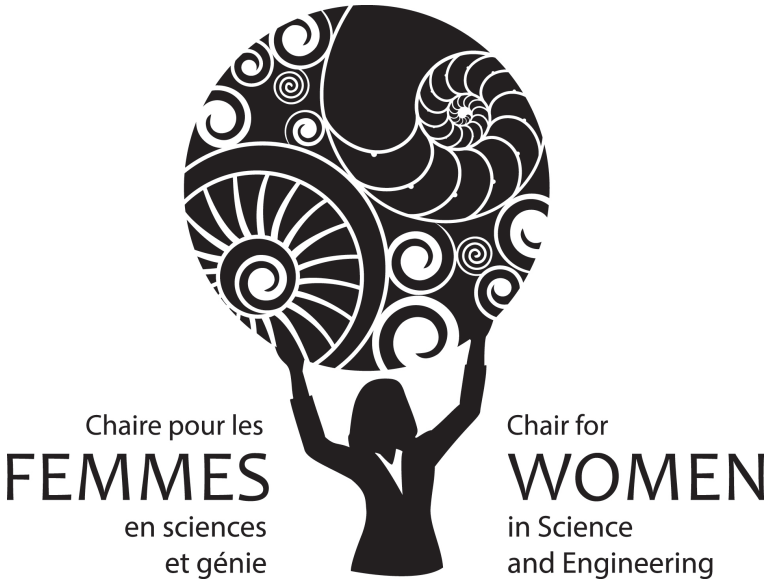
I will discuss my work in advancing women in science and engineering through US National Science Foundation funding since 1997 and, more recently, since 2011, Canada's Natural Sciences and Engineering Research Council Chair for Women in Science and Engineering program. The FORWARD to Professorship program, in particular, has been a successful vehicle to empowering doctoral women who consider academic careers. Results of a survey of all 1300 FORWARD participants since 2003 will be presented, giving a picture of how this group of talented and motivated women are advancing and how the climate is changing. My work in Canada has also included women in industry, in particular with the Chair sponsor, Pratt & Whitney Canada, an aircraft engine manufacturer based in Montreal. I will discuss activities designed for mid-career professional women in industry as well as some initiatives for boosting numbers of women in computing.



Interdisciplinary Conference Series:
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Surface-enhanced quantum control: A SEQC way of controlling light and matter

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Miniaturization of quantum technologies have led to the marriage of atomic physics and nanomaterial science. Some of the resulting new areas of research are hybrid quantum devices, single-molecule spectroscopies, table-top intense field generators, etc. I will present an area of research that I dub "Surface-enhanced quantum control" that is an exciting way of controlling light and nanomatter. By combining the electromagnetic enhancement properties of nanomaterials with the modification of the atomic properties, we can achieve an unprecedented level of control over quantum dynamics. I will present an example of surface-enhanced state purification.

This work was supported by an NSERC Discovery Grant. SMAM's Master's research and SG's co-op work term were partly supported by the NSERC Strategic Network on Bioplasmonic Systems. Computations were done on SharcNet supercomputers of the Compute Canada consortium.

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Computational Thinking and Simulations in Teaching Science and Mathematics

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We learn characteristics of scientific phenomenon conceptually. Using mathematical tools in science and engineering we can develop our conceptual understanding but computational thinking [1] and modelling with simulations can result in complete – more advanced understanding of scientific concepts, thus offering effective learning experience at different levels of education. In this work, we show how a simulation tool along with a mathematical one can be used to unfold the abstract side of science through visualization and project based introduction to science in fun and engaging ways for high school and first year university students. It can be effective approach in attracting young talented students, particularly more female students to science and technology by motivating their natural imagination to pose scientific abstraction.

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Fibre bundle framework for quantum fault tolerance

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Since it's a mathematical audience, I will start by giving a mathematical characterization of quantum error correction and fault tolerance, just what we need to understand this talk. We introduce a differential geometric framework for describing families of quantum error-correcting codes and for understanding quantum fault tolerance. In particular, we use fibre bundles and a natural projectively flat connection thereon to study the transformation of codewords under unitary fault-tolerant evolutions. We'll explain how the fault-tolerant logical operations are given by the monodromy group for the bundles with projectively flat connection, which is always discrete. Time permitting, we will discuss the construction of the said bundles for two examples of fault-tolerant families of operations, the string operators in the toric code and the qudit transversal gates.

Contributed Sessions

Applied Problems and Methods in Research & Education (CS-AMPRE)

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Exceptional Orthogonal Polynomials and Non-linear algebras associated with Quantum systems

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Last few years have witnessed a considerable level of research activity in the field of Exceptional Orthogonal Polynomials(EOP's) [1, 2, 3] which are new complete orthogonal polynomial systems and these are first observed as a result of the development of a direct approach to exact or quasi-exact solvability for spectral problems in quantum mechanics that would go beyond the classical Lie algebraic formulations. We have discovered new EOP families associated to such kind of systems in the regime of Supersymmetric Quantum mechanics. We have studied thoroughly some fundamental properties of those EOP families. More importantly, it is formidable job to prove EOP families are complete in weighted Hilbert space. We have been able to prove completeness of few such EOP categories in weighted Hilbert space, associated with the solutions of certain conditionally exactly solvable potentials obtained via unbroken as well as broken supersymmetry. Some other important key properties of such polynomials like recurrence relation, Rodrigues formula, ladder operators, differential equations etc. have been obtained. For instance, below we present a EOP family.

$$p_n(r^2) = \left[\frac{u'(r^2)}{r} L_n^{\alpha}(r^2) + 2u(r^2) L_n^{\beta}(r^2)\right] \tag{1}$$

where

$$u(r^2) = {}_1F_1\left(\frac{1-\varepsilon}{2}, \eta, -r^2\right) \tag{2}$$

and α, β, ε, η are parameters.

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Analytical Methods in Differential Equations, Optimal Control and Game Theory: An Educational Approach

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In this talk I will emphasize the utility of analytical methods that have been published in the area of the application of optimal control and game theory to life science, business and economics [1, 2]. Within this field of application, analytical methods of nonlinear optimal control have the benefit of tractability and interpretability over the conventional numerical methods through the type structures associated with switching functions which yield in a natural way to game-theoretic analysis.

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Growth Modeling of Mobile Communication Systems Adaptation in Learning

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There is increased interest/excitement among students who use mobile communication systems on our campuses. The ratio of students who have mobile phones to those without phones in an ideal class is 38:2. The availability of these mobile communication systems among our students either provide great potentials for increased learning if properly utilized or constitute nuisance to the learning system. This research seeks to discover and develop a model that will predict the level of adaptation of mobile communication systems in learning in our tertiary institutions and as well determine the effect/influence of such system on the academic performance of the students. Questionnaires were randomly distributed to students at various levels in our college and the information gathered was analyzed. Applying the Logistic Growth model on the data, a mathematical model

$$p = \frac{N}{1+5.67\left(e^{-0.58t}\right)} \tag{1}$$

where (N = sample size, t = time period in years)

for predicting the adaptation of mobile communication systems in learning within any given period was developed. Conclusion and appropriate recommendations are made.

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Learning Performances Assessment Models for Online Collaborative Learning Systems

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As the quest for collaborative e-learning continues to grow due to increase in the number of students en rolling in various academic programmes in our higher institutions, learning performances models for colla borative online learning environment that provide equal and credible assessment opportunities for all cate gories of learners in web-based learning environment have therefore become inevitable. Our mathematical models are developed with features for measuring level of class participation among students and instructo rs in online sessions of a course, their performances in collaborative studies; tests, assignment, polls and fi nal examination in a web-based learning environment. Objects used in developing the models include Instr uctor (I_k), course ($\mathbf{CO_k}$), student (S_j), Assessment ($\mathbf{A_{z,k}}$) and learning performance ($P_{k,j}$).
A particular student's learning performance in a particular course's online sessions is:

$$P_{k,\,j} = g_{k,\,j}(CO_k, S_j) + G_{k,\,j}(A_k) \quad (1)$$

Where:
$\boldsymbol{CO_k}$ represents courses offered in the WebVCS, $k = 1. ....n$ is the total number of registered online courses . (k is the course a student is participating)

$$g_{k,\,j}(CO_k, S_j) \quad (2)$$

represents a function that returns the weight of a particular student's participation in collaborative/group st udies of a particular course $\boldsymbol{CO_k}$.

$$G_{k,\,j}(A_k) \quad (3)$$

represents a function that returns the weight of a particular student's performance in a particular course $\boldsymbol{CO_k}$'s other forms of assessment (Attendance, Test, assignment, Polls).
The weight or value returned by $G_{k,\,j}(A_k)$ is a cumulative value computed as follows:
For a particular course $\boldsymbol{CO_k}$

$$A_k = \sum_{z=1}^{4} A_{k,z} \quad (4)$$

where:
z = 1,2,3,4 (z is assessment type), $A_{k,1}$ represents class attendance score, $A_{k,2}$ represents polls score $A_{k,3}$ represents score in assignment, $A_{k,4}$ represents score in test.
The learning performances assessment system model was implemented on windows 7 using MySQL rela- tional database management as backend engine, Hypertext Pre-processor (PHP) as frontend engine and Apache as web server. A case study of some level one students of Computer Science Department, Federal College of Education Kano was selected using course materials in different courses. The results obtained were validated, and analyzed to determine the efficiency and effectiveness of the system developed.

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Activity Recognition for Remote and Self-monitoring using Android Smartphones

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Activity Recognition is the task of automatically identifying daily human activities such as walking, jogging, climbing stairs, sitting, and standing. It has recently become a very promising area of research, especially because of its potential use for Tele-rehabilitation, remote monitoring of patients and also for people who just want to maintain a healthy lifestyle. Moreover, as opposed to unfriendly wearable sensors, activity recognition is now possible on modern smartphones due to built-in accelerometer sensors. This provides patients, a user-friendly manner to be monitored at a distance, just by keeping their phones in their pockets. In order to achieve this, CPU resource consuming machine learning classifiers are required. Previous researched work in this domain does prove that human activity recognition on mobile phones is possible with good accuracy but it concentrates on processing the sensor data on remote workstations over a network or offline (just for research purposes) without providing much practical use. A solution could be sending raw accelerometer data to a server for classification, but unreliable network issues results in data loss. A continuous need for a network connection also drains the battery by at least one-third. However, due to the high computing power of ubiquitous modern smartphones, the task is now possible within the smartphone itself in approximately real-time. A very few researchers who have implemented this approach, have struggled with achieving high accuracies for the activities. Another problem is to prevent the user from fooling the system by deliberate motion of the phone in his/her hands. This could be prevented by distinguishing between phone movement in the pocket and in the hand. This project focuses on the former problem – which is to develop a seamless mobile application that incorporates real-time activity recognition for continuous monitoring on the phone and has a high recognition rate. For this project, an Android application has been developed that recognizes walking, running and being inactive (which includes sitting and standing) in approximately real-time with an accuracy of 96.27%. The mobile application also shows calories expended for the respective activities, allows users to enter their weight goals and gives feedback to the user accordingly. Thus, the application acts as a self-fitness monitoring tool too. Such an Android application is novel.

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Optimal designs for heteroscedastic accelerated life testing models with multiple factors

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Accelerated life testing (ALT) provides a means of obtaining data on product lifetime and reliability relatively quickly by subjecting products to higher-than-usual levels of stress factors. In many situations, it is desirable to consider more than one stress factor. A lifetime distribution as well as a life-stress relationship are assumed and extrapolation is used to estimate percentiles of product lifetime at regular usage conditions. ALTs are often censored. Under a censored ALT, the resulting regression estimation problem becomes non-linear and usual least-squares estimation is not strictly applicable and so maximum likelihood estimation has been used.

Moreover, further savings can be obtained from good experimental designs. An experimental design specifies the levels of each stress factor (stress factor combination) and the proportion of test units assigned to each stress factor combination. Commonly used designs consist of equally spaced stress factors combinations, with the same number of units at each combination. Such designs are usually inefficient. An optimal design yields data that provide the most precise estimates among all the designs with the same number of test units and the same amount of test time.

There is extensive literature on optimal designs for single-factor ALTs, while very few on optimal design for multi-factor ALTs. Escobar and Meeker [1] showed how to design a two-factor ALT with *homoscedasticity*. However, it had been known for some time that the homoscedasticity assumption is often unreasonable and so Meeker and Meeter [2] gave a method for finding optimal designs for a *one-factor* ALT with *heteroscedasticity*.

In this paper, we present methods for finding optimal designs for two-factor ALTs for estimating percentiles of product lifetime, with time-censoring and heteroscedasticity. An outline of our results is as follows: (1) We generalize the method of Escobar and Meeker [1] to finding optimal designs for two-factor ALTs with heteroscedasticity; (2) we state and prove a result that for a special case, the method for homoscedasticity can be applied in the presence of heteroscedasticity to yield optimal designs; (3) we illustrate our methods using two practical examples treated in [1], but now assuming heteroscedasticity; we focus on the case when the parameters in the scale-stress relationship are not prespecified; (4) we present a brief comparison study and provide practical recommendations.

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Troeschs problem: Numerical simulation based on Haar wavelet collocation method

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In this paper, we develop an efficient numerical method based on uniform Haar wavelet method for the simulation of Troeschâs boundary value problem arising in the investigation of the confinement of a plasma column by radiation pressure. Through this simulation, solutions are found on the coarse grid points and refined towards higher accuracy by increasing the level of the Haar wavelets. More accurate solutions have been obtained by wavelet decomposition in the form of a multiresolution analysis of the function. The convergence analysis of Haar wavelet method is discussed and it is shown that error is inversely proportional to the level of the Haar wavelet. To demonstrate the accuracy of the proposed method a number of test problems are discussed. It is observed that the results obtained by this method are quite satisfactory and accurate, and the method is applicable for a wide range of cases when compared with existing solutions.

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Infinite families of (non)-Hermitian Hamiltonians assocoated with exceptional X_m Jacobi polynomials

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The classical orthogonal polynomial systems (OPS) of Hermite, Laguerre and Jacobi are most often characterized as the polynomial solutions of a Sturm-Liouville problem, following the celebrated result by S. Bochner: if an infinite sequence of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ satisfies a second order eigenvalue equation of the form

$$p(x)P_n'' + q(x)P_n' + r(x)P_n(x) = \lambda_n P_n(x), \qquad n = 0,1,2,\ldots \tag{1}$$

then $p(x), q(x)$ and $r(x)$ must be polynomials of degree $2, 1$ and 0 respectively [1]. In addition, if the $\{P_n(x)\}_{n=0}^{\infty}$ sequence is an OPS, then it has to be (up to an affine transformation of x) one of the classical orthogonal polynomial systems of Jacobi, Laguerre or Hermite. In recent years there is a surge of interest in exceptional orthogonal polynomials introduced in the seminal paper by Gomez-Ullate et al [2]. The exceptional X_m orthogonal polynomials (EOP) are the solutions of second-order Sturm-Liouville eigenvalue problem with rational coefficients. A distinguishing property of these polynomials is that the lowest eigen polynomial of the sequence need not be of degree zero, even though the full set of eigenfunctions still forms a basis of the weighted $\mathscr{L}^2$ space.

Motivated by the importance of orthogonal polynomials associated with exactly solvable quantum mechanical systems, the objective of the present work [3] is (using an appropriate change of variable) to transform the Schrödinger equation into a second-order differential equation satisfied by recently discovered Jacobi type X_m exceptional orthogonal polynomials. This is found to facilitate the derivation of infinite families of exactly solvable Hermitian as well as non-Hermitian trigonometric Scarf potentials and finite number of Hermitian and infinite number of non-Hermitian $\mathscr{P}\mathscr{T}$-symmetric hyperbolic Scarf potentials. The bound state solutions of all these potentials are associated with the aforesaid exceptional orthogonal polynomials. These infinite families of potentials are shown to be extensions of the conventional trigonometric and hyperbolic Scarf potentials by the addition of some rational terms characterized by the presence of classical Jacobi polynomials. All the members of a particular family of these 'rationally extended polynomial-dependent' potentials have the same energy spectrum and possess translational shape invariant symmetry.

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Mathematical Modeling of Glassy-winged Sharpshooter Population Dynamics

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Pierce's Disease (PD) is a bacterial disease of grapevines which is transmitted by xylem-feeding insects. PD can kill vines in one year with a serious threat to California and Texas wine industries. A database of the xylem-feeding insect population frequencies was collected by USDA-APHIS for Texas vineyards over multiple years. An initial statistical analysis of the data showed that the Glassy-winged sharpshooter (GWSS) had the greatest frequencies across Texas and was the most ecologically flexible [1]. This research focused on the GWSS frequencies within 25 vineyards located in central Texas. This study was supported in part by a NSF grant, which enabled two undergraduate students to participate in developing the mathematical model. The goal of the research was to investigate the natural population dynamics and decline of GWSS as the result of pest management campaigns on the insects within the region over the time period of years. We use a delay Gompertz model with harvesting and immigration terms:

$$\frac{dN}{dt} = -rN(t)\ln\frac{N(t-\tau)}{K} - cN(t) + I, \tag{1}$$

where r is an intrinsic growth rate, K is a carrying capacity and τ is a time-delay. For simplicity we assume that $c > 0$ and I is real numbers. The data is used to determine optimal values of parameters of the model based on a weighted least squares error function which accounts for multiple zeros in the data. The model gives us the predictive power to determine the impact of human intervention on controlling a disease and to what minimal level of the intervention required. Our future plan is to consider an optimal control problem where the harvesting term would be a function of time.

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Mathematics and Computation in Biological Sciences and Medicine (CS-BSM)

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Modeling and Simulation for the Effect of Beta Amyloid Aggregates on Acetylcholine Neurocycle through Choline Leakage Hypothesis

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A mathematical model is developed for studying the effect of Beta Amyloid (βA) and the Acetylcholine (ACh) neurocycle through two-enzyme/two-compartment model built previously by Mustafa et al., (2009) and choline leakage hypothesis developed by Ehrenstein et al., (1997). The presynaptic neuron is considered as compartment 1 while both synaptic cleft and the postsynaptic neuron are considered as compartment 2. It is found that as the feed βA increases in the presynaptic neuron, the choline content required synthesizing ACh decreases due to the leakage through the presynaptic membrane. Furthermore the concentration of βA increases until certain levels with time and increases with the increase of inlet βA concentrations.

Furthermore, not only the rate of ACh synthesis catalyzed by the enzyme ChAT in compartment 1 decreases but also the rate of the Ach hydrolysis in compartment 2 catalyzed by the enzyme AChE. Therefore, both ACh level in presynaptic neuron will decrease and ACh level in postsynaptic neuron decreases also due to the lack of ACh transport from compartment 1. However, the acetate concentration in presynaptic 1 decreases due to the accumulation and low consumption by ChAT, however Acetate levels in compartment 2 decrease due to the decrease in ACh levels in the postsynaptic neurons. pH in both compartments have been affected clearly to be outside of the physiological range. The reduction of both choline and ACh induces production of βA. The results are in agreement with the theoretical and experimental results and reflect the dangerous effect of βA aggregates leading to Alzheimer's and Parkinson's diseases.

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Nonlinear Robust Control and Regulation problems for Biomedical Dynamical Systems

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Motivated by topics and issues critical to human health and, safety and efficacy of medical treatment practices, this communication investigates a nonlinear robust control approach of some uncertain biomedical complex systems described by a class of nonlinear partial differential equations. The concept consists in setting the problem in the worst-case disturbances which leads to the game theory in which the controls and disturbances (which destabilize the dynamical behavior of the system) play antagonistic roles. The proposed strategy consists in controlling these instabilities by acting on certain parameters and data to maintain the system in a desired state (details of our approach are reported in Book [2]).

The real-time control and robust stabilization problems are formulated, in different situations, in order to reconstitute simultaneously different parameters, data functions and sources appearing in the state system and in the boundary conditions, and to control the online desired states provided by radiometric measurements (e.g., blood glucose, temperature). This work includes results concerning the existence of optimal solutions, sensitivity problems, adjoint problems, necessary optimality conditions (necessary to develop numerical optimization methods) and optimization problems. This approach is applied to two problems (Refs [1, 3, 4, 5, 6]): first, controlling and regulating the blood glucose level in subjects with type 1 diabetes and predicting the dosages of insulin administered, and second, controlling and stabilizing the thermal dose distribution in tissue and damage during laser-induced interstitial thermotherapy (often used in the treatment of cancer), in order to eradicate tumor while preserving the surrounding health tissues.

Some numerical strategies, based on adjoint control optimization, in order to perform the robust control, are also discussed.

keywords : Robust control, stabilisation, regulatory system, biomedical systems, cancer, diabetes, adjoint model, necessary conditions of optimality.

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Role of predators in dynamics of niche construction

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In the work [1] a question of "how much overconsumption a renewable resource can tolerate" was addressed using a mathematical model "resource –consumer population" [2], where consumers had realized a strategy of their environmental capacity increasing and individuals in a population not only compete for the common resource, but can also contribute to its restoration. A threshold of the system resistance to over-consumers (individuals that take more than they restore) was found by the bifurcation analysis of the model; a series of transitional regimes that the population goes through before it exhausts the common resource and thus goes extinct itself (a phenomenon known as ''the tragedy of the commons'') was identified. The results of the model analysis were formulated with help of analytical and numerical construction of the bifurcation diagram; six phase-parameter domains corresponding to qualitatively different model behaviors were revealed. It was also observed that (1) for some parameter domains a population can survive or go extinct depending on its initial conditions, (2) when the natural decay rate of the common resource is high enough, the population can endure the presence of more aggressive over-consumers without going extinct.

In this work we generalized the recent model proposed in [2]. In scaled variables N (preys), p (predators), z (resource) the model is of the form:

$$\begin{cases} \dfrac{dN}{dt} = N(c - \dfrac{N}{z} - \dfrac{p}{\alpha + N}), \\ \dfrac{dp}{dt} = \beta p(N - m), \\ \dfrac{dz}{dt} = \gamma - \delta z + \dfrac{e(1-c)N}{N+z} \end{cases} \tag{1}$$

where $c, e, \beta \le 1, m, \alpha$ are the Malthusian coefficient of prey growth, a coefficient of the transformation of preys to predators biomasses, a level of coexistence of predators and preys and a caring capacity coefficient of the prey population, γ, δ characterize level of natural resource restoration and its decay.

We show that a suitable "choice" of predator can preserve resource and preys. The possible applications of the model are also discussed.

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A spatial computer model for the spread of hepatitis C virus infections in vitro

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Mathematical and computer models that reproduce the spread of a viral infection within a cell culture (in vitro) provide unique, valuable information: the accurate quantification of key infection parameters (e.g., viral production rate, infectious cell lifespan). Changes in these parameters, in turn, can indicate how a mutation affects viral fitness or identify the mode of action and efficacy of novel antiviral drugs.

There currently exists only one mathematical model describing the course of a hepatitis C virus (HCV) infection in vitro: a non-spatial ODE model [1]. However, experiments have shown that the spread of HCV infection has an important spatial component: infection disseminates both distally via release and diffusion of virus through the medium, and locally via direct, cell-to-cell infection [3]. Both infection modes appear to play an important role, yet these two routes of infection could be differentially affected by antiviral therapy. Therefore, characterizing their relative contribution to infection kinetics has important implications for the control of HCV infections.

We have developed an agent-based computer model which explicitly incorporates both of these infection routes. The model consists of a two-dimensional, hexagonal grid in which each site corresponds to one, non-motile, hepatocyte (liver cell). Since experimental measures taken over the course of the infection typically report both the concentration of infectious virus in the medium bathing the cells (extracellular), as well as the count of virus RNA segments within infected cells (intracellular), our model also tracks both of these quantities. Within each cell, the concentration of HCV RNA is tracked and updated via an ODE model for intracellular viral replication [2]. The intracellular concentration within each cell is, in turn, linked to both the rate at which a cell will release extracellular virus and the rate at which the infected cell causes infection of its immediate neighbours.

In this presentation, I will showcase the range of kinetics exhibited by our model and its performance in reproducing measurements from actual experimental in vitro HCV infections.

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Modelling 1, 5 and 10 µm Particle Deposition In Human Lung By CFD

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The particle deposition in human lungs has been studied recently. Because it is a biological system that is complicated to investigate experimentally, Computational Fluid Dynamics (CFD) is an alternative to study how inhalable particles deposit in the airway bifurcations. In this work, a tridimensional triple airway bifurcation corresponding to generations 3rd to 6th, in which airway diameters range from 0.29 to 0.6 cm, was used (Figure 1).

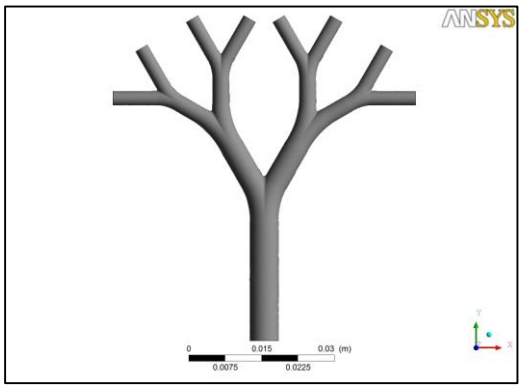

Figure 1: Tridimensional lung airway bifurcations.

The transport equations were solved for steady-state, laminar and isothermal flow, at 310.15 K. The particles have diameters equal to 1, 5 and 10 µm and 1000 kg/m³ of density. To describe the gas and particles phases, respectively, the Eulerian-Lagrangian approach was used. Three different entrance flow rates of 15, 30 and 60 L/min in the trachea were considered to represent situations of rest, moderate activity and heavy activity. To represent the fluid-particle interaction, the one-way coupling method was used. That is resonable because the particle concentration is low and the particle diameter is considered small. Inertial and gravitational deposition were considered, leading to the force balance that describes the particle:

$$\frac{d}{dt}(m_p \mathbf{v_p}) = \mathbf{F_D} + m_p \mathbf{g} \qquad (1)$$

where m_p is the mas and v_p is the velocity of the particle, $\mathbf{F_D}$ is the drag force and $\mathbf{g}$ is gravity acceleration.

The Commercial software ANSYS 14.0® was used to run the simulation. The mean Stokes number values were smaller than 1, indicating that most particles follow the stream lines of the air flow. The results were compared with experimental data from the literature and showed that the model was capable of representing the particle deposition. Thus, the results of this work indicate that CFD is a viable and important tool for studying particle deposition in human airway bifurcations and can be used for optimization of devices for inhalable drugs.

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Singular perturbation solutions of steady-state Poisson-Nernst-Planck systems

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We study the Poisson-Nernst-Planck (PNP) system with an arbitrary number of ion species with arbitrary valences. Assuming that the Debye length is small relative to the domain size, we derive an asymptotic formula for the steady-state solution by matching outer and boundary layer solutions. The case of two ionic species has been extensively studied, uniqueness of the solution has been proved and an explicit expression for the solution has been obtained. However, the case of three or more ions has received significantly less attention. Previous work has indicated that the solution may be non-unique and that even obtaining numerical solutions is a difficult task since one must solve complicated systems of nonlinear equations. By adopting a methodology that preserves the symmetries of the PNP system, we show that determining the outer solution effectively reduces to solving a single scalar transcendental equation. Due to the simple form of the transcendental equation, it can be solved numerically in a straightforward manner. Our methodology thus provides a standard procedure for solving the PNP system and we illustrate this by solving some practical examples. Despite the fact that for three ions, previous studies have indicated that multiple solutions may exist, we show that all except for one of these solutions is unphysical and thereby prove existence and uniqueness for the three ion case.

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Designing of Mathematical Models in the Study the Essential Hypertension among the Euglycemic Patients of Ischemic Heart Disease

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For the study of Hypertension, two mathematical models have been designed to measure the main effecting factors SBP and DBP depending on independent factors, body mass index, tri-glyceride, low density lipoprotein- cholesterol and high density lipoprotein-cholesterol. Adequacy of the models has been verified using analysis of variance (F-test), histogram, Q-Q plot and box whiskers plot methods. It has been shown that body mass index; tri-glyceride, low density lipoprotein- cholesterol and high density lipoprotein-cholesterol are the main factors affecting the SBP and DBP significantly. It has also been shown that TG and BMI are more affecting the blood pressure as compared to other factors. The graphs have also been plotted corresponding to fitted models and original data which show that fitted models are best models to obtain the values of SBP and DBP. An effort has been made to analyze the data and interpret it with the help of statistical software package SPSS 14.0.

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Non-Linearity and Heterogeneity in Modeling of Population Dynamics

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E. Szathmary and M. Smith ([1]) represent the model of prebiological evolution of replicators by the "power" equation for the concentration of molecules

$$\frac{dx}{dt} = kx^p \quad (1)$$

Three cases are distinguished: the exponential with $p = 1$; the super-exponential (hyperbolic) with $p > 1$; the sub-exponential (parabolic) with $p < 1$. The models of biological populations composed from non-exponential *homogeneous* subpopulations (clones) demonstrate deviation from Darwinian "survival of the fittest", see [1], [2] for discussion. Nevertheless, both hyperbolic and parabolic growth can be observed in real populations at large enough domains of the model variable values. Well established examples of non-exponential growth apply to global demography with p=2 [3] and some molecular replicator systems with p=1/2 [4]. The question arises: what are possible origins of the non-exponential models and how to derive them from realistic assumptions?

We consider the power equation within the frameworks of inhomogeneous population models with distributed Malthusian parameter [5] and prove that the equation (1) $\frac{dN}{dt} = kN^p$ for any $p > 0$ describes the total population size of inhomogeneous frequency-dependent model

$$\frac{dl(t,a)}{dt} = \frac{kal(t,a)}{N(t)} = kaP(t,a),\ N(t) = \int_A l(t,a)da \quad (2)$$

where the initial distribution of the parameter a, $P(0,a)$, is the Gamma-distribution.
We study also a general frequency-dependent population model (2) with arbitrary initial distribution of the Malthusian parameter and prove that this inhomogeneous model demonstrates Darwinian "survival of the fittest" if and only if the moment generating function $M(\lambda)$ of the initial distribution of the Malthusian parameter is finite for all λ. In other case the model demonstrates non-Darwinian "survival of everybody".

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Optimal Control of Bioheat Equation using Semigroups

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A distributed optimal control problem for a system described by a bioheat transfer equation for a homogeneous skin is analytically investigated using strongly continuous semigroups. The required skin temperature at a specific depth point is attained within the total operation time due to microwave radiation which is taken as a control. A novel numerical method based on semigroup theory is proposed. Controllability and stability is investigated. Numerical results are presented with some examples.

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A Model of Clusters in Binary and Ternary Strings Applied to Protein Secondary Structure Prediction

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Efficient and reliable prediction of protein secondary structures is an important and well developed area in Computational Biology. State of the art methods achieve a standard Q_3 score greater than 75%. Ultimately, all of them rely heavily on vast databases of experimentally observed secondary structures and known proteins' homologs; and they use this data with remarkable success! Nevertheless, the problem of secondary structure prediction is still far from being solved, and there is a room for new ideas and approaches. In this work, we make a new attempt to move away from data-driven methods, and revisit the problem from a solely mathematical perspective.

We approach the problem by associating each of 20 common amino acids with either 1 or 0, so that 1s represent "structure formers" (discussed later), and 0s are indifferent residues. This amino acid classification transforms the residue sequence of a protein into a binary string. Knowing naturally occuring probabilities of different amino acids, we can compute the probabilities of 1s, denoted by p, and 0s, $q = 1 - p$.

For a given 1, our algorithm looks for the most probabilistically *rare* (henceforth "the best") cluster of 1s that contains it. We introduce a cluster connectivity distance $k \geq 0$ such that two 1s are in the same cluster if they within a distance not more than k; k can be different for different clusters. Conceptually, this model extends Percolation Theory on a line by allowing connections between nodes that are not immediate neighbors.

We prove that, on infinite strings, the search for the "best" cluster for a given 1 necessarily fails with probability 1 as k increases. Thus there is a need for "breakers", the third class of amino acids denoted by symbol π, which stop cluster growth (they are equivalent to an infinite string of 0s). If the probablity of breakers is non-zero, the "best" cluster always exists. By running the algorithm on all 1s in a sequence, we obtain a nested hierarchy of clusters (some clusters with smaller k are contained in others), and then, using a simple heuristic that relates k to the periodicity of secondary structures, merge this hierarchy into a prediction string, i.e. every residue is said to belong to a "helix", "strand", or "coil". This prediction string can be matched against the corresponding database record to determine prediction accuracy.

To identify correct "structure formers" and "breakers", we use the DSSP database which includes annotations of secondary structure of proteins. With the Q_3 score serving as a fitness function, we run a genetic algorithm to find the best mapping of each of the 20 amino acids to 1, 0, or π. In several variants of the algorithm, the mapping of hydrophobic amino acids to 1 and $\{P,G\}$ to π is consistently obtained, which is in agreement with biological properties of amino acids. The score $Q_3 = 55\%$ is reached for the standard CB-513 dataset, which is better than comparable Chou-Fasman and GOR methods (and their variants). Therefore, with just minimal data extracted from the database (the mapping), we are able to obtain reasonable performance. The consistency of the mapping suggests that our mathematical model conforms with whichever evolutionary mechanism lead to the formation of biological structures. To substantiate this further, we run simulations on random sequences, iteratively updating the probabilities of 1, 0, and π based on their occurence in the found clusters in a way similar to Bayesian learning. The simulations converge to the typical probabilities found in amino acids sequences.

We believe our work can be invested further to develop algorithms for structure identification (not necessarily biological) that move away from the data-driven approaches.

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Modeling Blood Flow in a Brain Tumor Treated Concurrently with Radiotherapy and Chemotherapy

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Objective: Many brain tumors are highly invasive and therefore extremely difficult to treat [1-3]. Many studies have demonstrated a better outcome with concurrent application of radiotherapy and chemotherapy. Our major objective in this paper is to understand the physiology of blood flow in a solid tumor, and also to investigate the effect of concurrent application of two anticancer drugs in a solid tumor.

Status: We investigated the charactertics of unsteady blood flow within an unsteady homogeneous tumor. We presented results for the unsteady cases including, specifically, those affected by the growth rate of the tumor and how much the growth rate can be controlled by drug delivery mechanisms. In future, we will extend our present model and apply it to nonunidirectional tumors and tissues in terms of properties and geometrical configurations.

Methodology: A coupled convection-diffusion-reaction model for simulating interaction between two anti cancer drugs has been developed. This model provides the computational transportation to evaluate systematically and quantitatively the effects of interaction between two drugs.

Results: We found that the interstitial pressure is the maximum at the center of the tumor core, while the magnitude of the interstitial velocity is the minimum at this point. The concentration of two anticancer drugs is higher at the center of the tumor and increases faster than the border region with time. The concentration is higher in a tumor when there is an interaction between the two drugs than without interaction. As the growth rate of the tumor increases the magnitude of the concentration decreases

Significance: Combining mathematical models with clinical research is definitely a new way of thinking about oncology. In this paper we have presented some promising modeling approaches to simulate the radiotherapy and chemotherapy response of cancer cells and whole tumors. Our mathematical models are developed in close observation of clinical data, and hence this model can prove to be vital in augmenting current biological and clinical radiotherapy and chemotherapy knowledge.

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Modeling Oxygen Dynamics of the Retina - Using Discrete Exterior Calculus

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Open Angle Glaucoma is a multifactorial optic neuropathy characterized by progressive retinal ganglion cell death and associated visual field loss. The medical community found evidence that alterations in blood flow effect disease processes, but until now only few detailed physical models exist for the eye. We model blood pressure in the retina of the eye by solving Darcy flow equations for non-homogeneous porous media on a flat circular surface and on a hemispherical surfaces with appropriate boundary conditions. We compare the distribution of pressure and velocity. Our study shows that ocular curvature has a noticeable effect in pressure distribution, which suggests that alterations in ocular curvature, such as those occurring in myopic eyes, might contribute to glaucomatous damage by reducing retinal blood flow.

To solve the problems we use discrete exterior calculus and finite element exterior calculus. Exterior calculus developed by Cartan several decades ago has gradually been gaining acceptance as the superior formulation of vector calculus. Its main advantage is coordinate independence which makes these methods very suitable for problems on curved surfaces. The language of exterior calculus shows the geometry of a problem (flow, curvature, symplecticity) and has led to the development of numerical methods which preserve geometrical structures (conservation of energy, symplecticity) of the original equations. We present the problem formulation in exterior calculus and discuss some aspects of exterior calculus on curved surfaces.

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Effect of boundary absorption on dispersion of solute in a pulsatile Casson fluid flow

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The present study analyses the effects of wall absorption on the dispersion process of a solute in a Casson fluid flow. Here we consider the flow is unsteady since the flow in the circulatory system is pulsatile due to heart pumping. The generalized dispersion model is used to study this process and according to this model the entire dispersion process is expressed in terms of three transport coefficients viz. absorption, the convection and dispersion coefficients. This model brings out the effects of pulsatility, yield stress and wall absorption on dispersion process in a Casson fluid flow. This model can be used to understand dispersion process in cardiovascular flows, in particular in drug delivery and oxygen transport.

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Dynamic models for rodent pest control: A case study of plateau pika

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The overabundance of plateau pika brings a great damage to the alpine meadow. Rodenticide and sterilant have been used to control this mammalian pest. In this talk, we propose models to incorporate these controls and the seasonal cycle of breeding and non-breeding. When the basic reproduction number is less than 1 then the trivial equilibrium is globally asymptotically stable; if the basic reproduction number is greater than 1 then the trivial equilibrium is unstable and there is a positive equilibrium which attracts all positive solutions. Larger contraception rate, larger lethal rate, and shorter control interval could have better control effects, which may make the controlled population become smaller and even die out. Short-acting sterilant limits the control effect and the controlled population would have a weak recovery at the later period of breeding season. These theoretical results are supported by numerical simulations. We also suggest possible strategies to be implemented in practice.

Computational Algebra, Combinatorics and Optimization (CS-CACO)

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Bias, Noise, and Indeterminacy Correction in Numerically Invariant Signatures

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Numerically invariant signatures were introduced as a new paradigm of the invariant recognition for visual objects modulo a certain transformation group. This paper illustrates that the current formulation in terms of joint invariants suffers from bias, noise, and indeterminacy in the resulting numerical signatures. The numerical biases which may arise in the resulting numerical signatures are classified as Bias Type-1 and Bias Type-2, and it is illustrated how they can be removed. Next, we apply the n-difference technique and the m-mean signature method to reduce the effects of noise and indeterminacy in the resulting outputs. In our experimental results of applying the proposed numerical scheme to generate joint group-signatures, the sensitivity of some parameters such as regularity and mesh resolution used in the algorithm will also be examined. Finally, several interesting observations are made.

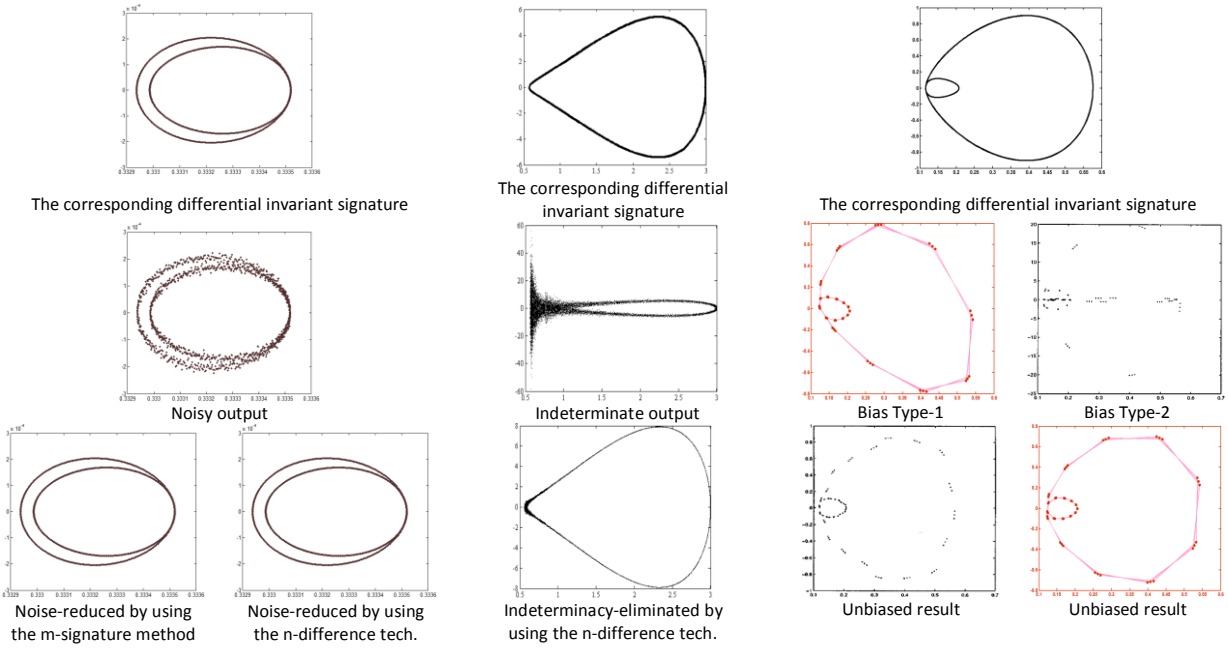

Figure 1: Illustrates bias, indeterminacy, and noise in the resulting numerically invariant signatures and how these issues can be removed.

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Design and Application of Fault-Tolerant Circulant Digraph Networks

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Fault tolerance is a major design goal in building multicomputer networks that must continue to operate correctly in the presence of faults. This is usually achieved by introducing redundancy to the network, that is, by adding spare nodes and links. In this case, when some of the basic components fail, the network can be reconfigured to bypass the defective parts and replace them with healthy components.

Building fault-tolerant systems has been examined for many architectures (such as rings, stars, tress, meshes, and hypercubes). In this work, we study this problem for the circulant digraph configuration. Moreover, we show how to apply our formulation to handle failures in some other networks whose edges are all undirected, or even mixed (i.e., some are directed and some are undirected). Circulant digraphs form an important class of loop-based architecture that has been applied to the design of many local area networks and some parallel computers (such as the ILLIAC machine).

The optimization criterion used in this paper is to reduce the node-degree of the overall network. This is an important objective in practice due to the limitation on the number of links allowed per node in a VLSI design. It is well-known that finding a fault-tolerant design that is optimal with respect to this criterion is generally very difficult even for networks with a regular structure.

The formulation proposed in this paper has many advantages. First, it is efficient to implement, and moreover, it can handle any number of node failures. In addition, the reconfiguration involved is simple and requires only a linear time (in the size of the network). Our results indicate that the (fault-tolerant) solutions we obtained are either optimal or nearly optimal.

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New Approach for solving the Linear Assignment Problem

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The linear assignment problem is a fundamental combinatorial optimization problem consisting in finding an optimal matching between two sets of equal dimension. An excellent illustration is the assignment of n jobs to n different workers with a variety of degrees of skill. The linear assignment problem has numerous applications in a large variety of domains such as production planning, scheduling, telecommunications, economics etc…
One popular solution method for the linear assignment problem is the Hungarian method. In this research, we introduce a new iterative solution method by applying the Vogel Approximation Method (VAM) to the problem's reduced cost matrix. At each iteration, one assignment is performed using the VAM, the corresponding line and column are simultaneously removed from the matrix cost leading to a smaller assignment problem to be solved. A certain number of rules are provided to eliminate the need to recalculate a new reduced cost matrix for the new assignment problem. This approach seems to provide an easiest way to find some independent zeros than the Hungarian Method. And, unlike the VAM for transportation problem, the algorithm converges to the optimal solution. Numerical tests are performed using Java.

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Solving the simple Transportation Problem by using the Modified Vogel Approximation method

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The Vogel method is one the methods which provide starting basic solution to the transportation algorithm. Moreover, it is an approximation method and therefore called Vogel Approximation Method (VAM). In this presentation, we introduce a modified version which constitutes an improvement of the VAM for the transportation problem. This new approach called Modified Vogel method (MVM) consider the equivalent transportation problem defined by the reduced cost matrix. Then it applies the Vogel method to determine the variable to be assigned. After each assignment of a variable, the remaining matrix is reduced. A certain number of rules are provided to eliminate the need to recalculate a new reduced cost matrix for the whole remaining table. The Modified Vogel method (MVM) assigns, in some cases, simultaneously a bundle of variables. In the case where all the penalties were zeroed, it provides the optimal solution. It also allows the identification of the optimal solution whenever the reduced cost equals to zero. Consequently this avoids, in these cases, the use of the transportation algorithm. Numerical tests are performed using Java.

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Highly Accurate Solution of Ordinary Diferential Equation with Singularity Arising in Fluid Dynamics

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A complex boundary value problem consisting of a second order differential equation with singularity, arising in fluid mechanics, is solved to high precision. The second order differential equation must be solved on $(0, \infty)$ subject to the boundary condition that specify the asymptotic behaviour of the solution at the two ends of the solution domain. The solution at the origin is expanded using analytic continuity and matched with the asymptotic solution. The solution is obtained by computing multiple series. To obtain a high accuracy, a large number of terms in each series is computed which is only possible by virtue of symbolic computation. All the routines for this purpose are developed in the symbolic computational package, *MAPLE*.

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Nondeterministic relational fuzzy operators

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The calculus of relations has been an important component of the development of logic and algebra since the middle of the nineteenth century. George Boole, in his "Mathematical Analysis of Logic" [3]. Schroder's work, however, lay dormant for more than 40 years, until revived by Alfred Tarski in his seminal paper "On the calculus of binary relations" [7]. Tarski's paper is still often referred to as the best introduction to the calculus of relations. The demonic calculus of relations [4, 6] views any relation R from a set A to another set B as specifying those programs that terminate for all $a \in A$ wherever R associates any values from B with a, and then the program may only return values b for which $(a,b) \in R$. Consequently, a relation R refines another relation S if R specifies a larger domain of termination and fewer possibilities for return values. The demonic calculus of relations has the advantage that the demonic operations are defined on top of the conventional relation algebraic operations, and can easily and usefully be mixed with the latter, allowing the application of numerous algebraic properties [1, 5, 8].

Fuzzy "As the complexity of a system increases, our ability to make precise and yet significant statements about its behavior diminishes until a threshold is reached beyond which precision and significance (or relevance) become almost mutually exclusive characteristics." [9]

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 of nondeterministic programs [2]. We deal with a relational algebra model to define a refinement fuzzy ordering (demonic fuzzy inclusion) and also the associated fuzzy operations which are fuzzy demonic join ($\sqcup fuz$), fuzzy demonic meet ($\sqcap fuz$) and fuzzy demonic composition ($\square fuz$). We give also some properties of these operations and illustrate them with simple examples.

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Computational Physics and Chemistry (CS-CPC)

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Properties of dimethylimidazolium chloride- monosubstituted benzene at T=400K

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Recently the more and more attention is paid to the investigation of properties of ionic liquids consisting from large inorganics cations and small organics anions. Such ionic liquids are of great practical importance for the chemical industry and other field of economies. One of the simplest representatives of the class of ionic liquids is dimthylimidazolium chloride (dmem+/Cl-) .

Investigations of the tree-component systems ionic liquids-molecule of the monosubstituted benzene we used various types potentials for description of inter- and intra molecular interactions. The calculation ware performed at the constant temperature T=400K for the ensemble consisting 192 cations, 192 anions and one dissolved molecule, with gave a possibility to estimate the influence of dissolved molecule (benzene, toluene, anisole or phenol) on the local structure of the ionic liquids in detail.

The work presents results on the local structure, the energy and dynamics characteristics in the case of the interactions of a monosubstituted benzene molecules (benzene, toluene, anisole or phenol) with the dimethylimidazolium chloride at T=400K calculated by molecular dynamics method. We established existence of the hydrogen bonds between a alcohol molecule (benzene, toluene, anisole or phenol) with dimethylimidazolium and chloride at T=400K and determinate the energy and dynamics characteristics three-components systems of the study.

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Thermodynamic and dynamic anomalies in a simple one-dimensional lattice model of water

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The behavior of the self diffusion constant of one dimensional lattice fluid models as a function of density and temperature was studied through computer simulations using the Monte Carlo method. Particle's dynamics were implemented using one- and two-site jumps. The proposed model is simple and, besides a hard-core, has a single a repulsive interaction between nearest neighbors. This model can be considered as a simpler version of other 1D models for water [1], which include an attractive first nearest neighbor and an attractive second nearest neighbor introduced to imitate the wider range of the hydrogen bond interaction. Theoretical calculations and simulation showed that, despite its simplicity, our model reproduces the anomalous behavior of water on the diffusion constant and on density, in a region corresponding to a "transition" between a dense fluid and a bonded fluid (BF-DF). We have also calculated the diffusion constant through an approximate analytical treatment based on a simple random walk. Computer simulations and theoretical results are being compared to check the range of validity of the simplifying hypothesis assumed theoretically.

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Adaptive Matrix Transpose Algorithms for Distributed Multicore Processors

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The matrix transpose is an essential primitive of high-performance parallel computing. For example, multidimensional fast Fourier transform algorithms rely on a matrix transpose to localize the computation onto individual processors. Historically, a number of different algorithms have been proposed for matrix transposition on distributed memory archictures. For instance, Choi *et al.* [3] identified, in order of increasing speed, the *rotation*, *direct communication*, and *binary exchange* algorithms. However, the relative performance of these transposition algorithms depends on many factors, including communication latency, communication bandwidth, network congestion, communication packet size, local cache size, and network topology. Since it is hard to estimate the relative importance of these factors at compilation time, an adaptive algorithm, dynamically tuned to take advantage of these specific architectural details, is desirable.

Al Na'Mneh *et al.* [1] have previously described an adaptive transposition algorithm for symmetric multiprocessors that share a common memory pool and exhibit low-latency interprocess communication. At the other extreme are adaptive algorithms optimized for distributed memory architectures with high latency communication, like those implemented in FFTW [4]. However, modern high-performance computer architectures consist of a hybrid of these two opposing models: distributed networks of multicore processors.

In this work, we describe recent efforts to exploit modern hybrid architectures, using the popular MPI message passing interface to communicate between distributed nodes and the OpenMP multithreading paradigm to communicate between the individual cores of each processor. One of the advantages of exploiting this hybrid parallelism is that it is often possible, through the use of a combination of memory striding and vectorization, to arrange applications of matrix transposes (such as multidimensional fast Fourier transforms) so that local transposition is not required within a single MPI node. While transposition algorithms do not normally benefit from multithreading, since the multicore nodes in modern hardware are typically connected to the distributed network via a single socket, the computational phases of the calling process usually does. The hybrid paradigm thus provides an optimal setting for nonlocal computationally intensive operations found in applications like the fast Fourier transform.

We apply adaptive matrix transposition algorithms on hybrid architectures to the parallelization of implicitly dealiased pseudospectral convolutions used to simulate turbulent flow. Implicit dealiasing outperforms conventional zero padding by decoupling the data and temporary work arrays. Parallelized versions of our implicit dealiasing algorithms for hybrid archictures are publically available in the open-source library FFTW++ [2].

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Theoretical Analysis and Iteration Acceleration of Second-order Temporal Accurate Fully Implicit Discretization for Nonlinear Diffusion Problem

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The fully implicit finite difference (FIFD) schemes with second-order temporal accuracy have been used to solve nonlinear diffusion problems for a long time [1], but there is seldom rigorous theoretical analysis for their accuracy. In this work, discrete functional analysis [2]is applied to analyze such an FIFD scheme for two-dimensional nonlinear diffusion problem, and Newton iteration acceleration is designed to solve the problem efficiently. To prove the convergent ratio and approximate accuracy of the Newton iteration in discrete functional analysis procedure, the $L^{\infty}(H^1)$ convergence property of the FIFD scheme is indispensable. Two methods are studied to provide such a convergence property. One follows an inductive hypothesis reasoning technique suggested by the authors in a recent paper [3], the other is a novel one, which completes the proof in two steps. First, with a thorough estimate of the terms corresponding to the discrete temporal derivative, the $L^{\infty}(L^2)$ convergence is proved. Then by using it in an inductive reasoning procedure, the difficulty arising from the nonlinearity is overcome, and the $L^{\infty}(H^1)$ convergence is proved. A complete theoretical analysis is obtained for both the FIFD scheme and the Newton iteration. It shows that the nonlinear FIFD scheme is absolutely stable, the Newton iteration converges with a quadratic ratio, and their solutions have second-order convergence both in spatial and temporal variants to the exact solution of the original problem. Numerical tests are provided to highlight the theoretical results and demonstrate the high accuracy and efficiency of the second-order time-accurate Newton iteration.

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The dynamics of the fluxion in curved Josephson junction

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The influence of the curvature of the long Josephson Junction on the dynamics of the fluxion is considered. On the base of Maxwell and Landau-Ginzburg theories the effective equation that describes the dynamics of the gauge invariant phase difference of the many-particle wave functions, that describe superconducting electrodes, is obtained [1]. The existence of the kink solutions in the effective (modified) sine-Gordon model is investigated. The movement of the fluxion in the framework of the sine-Gordon model is studied numerically. The dynamics of the collective coordinate that describes position of the kink is studied analytically. It is shown that the curvature of the junction corresponds to the existence of the potential barrier experienced by the fluxion [2].

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Avoiding the coordinate singularity problem in the numerical solution of the Dirac equation in cylindrical coordinates

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Due to recent and prospected technological advances, it is now possible, to consider laser intensities of 10^{23} W/cm^2 and higher. In this new regime, relativistic and quantum electrodynamics effects start to be important, requiring a theoretical description in terms of the time-dependent Dirac equation. In this presentation, I will present recent advances on the numerical solution of this equation for 3-D axisymmetric geometries using cylindrical coordinates. The numerical method is based on a split-step scheme in coordinate space, which is free from the "fermion doubling" problem and which can be parallelized very efficiently. A new technique to circumvent the coordinate singularity at $r = 0$ using Poisson's integral solution of the wave equation for the radial operator will also be described. The general strategy is to interpolate the solution using cubic Hermite polynomials and to integrate exactly the Poisson solution. The result of this procedure gives a non-standard finite difference scheme on a time staggered grid. The numerical method is then utilized to simulate the quantum relativistic dynamics of an electron bound in a diatomic molecule potential and interacting with an ultraintense counterpropagating laser field.

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Using Computational Chemical Methods to Gain Insights into the Enzymatic Mechanism of LuxS

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S-ribosylhomocystein (LuxS) is an enzyme that allows diverse bacterial species to communicate with one another. Importantly, many pathogens have been shown to possess LuxS[1], indicating its possible involvement in the spread of infections. The mechanism, by which LuxS operates, and its atomistic details remain unsettled. These are key prior to the development of pharmaceutical drugs that may inhibit LuxS and possibly stop the spread of superbugs. This study uses computational chemical methods to study in details the mechanism of LuxS. Specifically, we have used molecular dynamics (MD) simulations to model the motion of atoms within the enzyme and we have used QM/MM methods to calculate the kinetic and thermodynamic properties pertaining to its mechanism. Insights into subtrate binding, which can allow for subsequent rational drug design studies, have been obtained. On a broader scale, our results demonstrate how a combination of different computational chemical methods can be used to uncover the driving forces in enzymatic systems.

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Polarizability Calculations of Linearly Conjugated Systems Using Matrix Product States

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The matrix product states (MPS) approach is a new method for solving the many-electron Schrödinger equation recently implemented by Wouters *et al* [1]. This method is used to determine the static polarizability and second hyperpolarizability of polyacetylene chains with a fully active π-orbital space. Comparison of various active spaces revealed that the contribution of the active σ-orbitals is significantly less than that of the π-orbitals and thus can be neglected. The polarizabilities of polyacetylene systems ranging up to 16 double bonds were calculated with the finite field method using different basis sets and can now be used as an accurate benchmark for other methods. These results demonstrate for the first time that the benefits of MPS, well studied for small model systems, can be efficiently transferred to real chemical systems of substantial size.

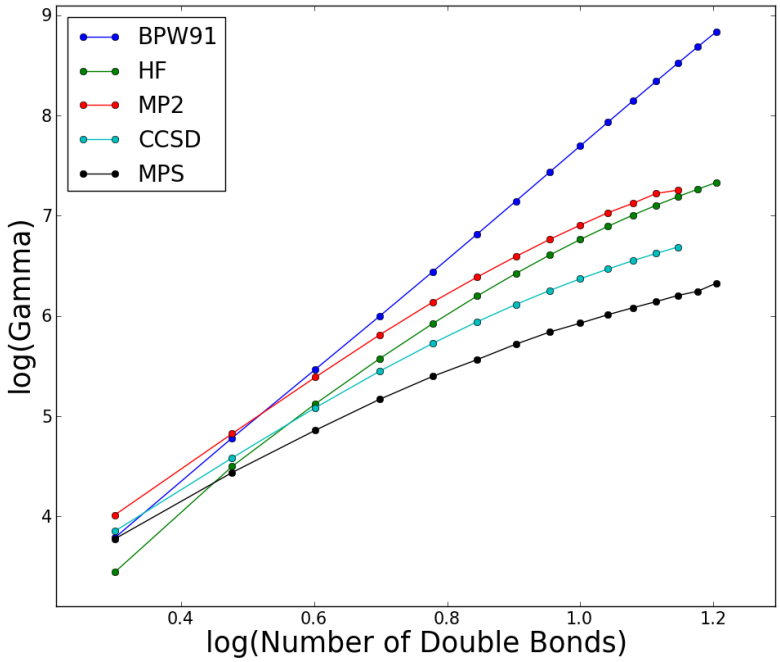

Figure 1: Calculation of second hyperpolarizability for polyacetylene systems using various methods and basis set STO-6G

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Constraints on "Rare" Dyon Decays

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Recent developments have given us a much better understanding of the degeneracy counting formula for 1/4 -BPS dyons in N = 4 string compactifications. This formula has been considerably refined from its original form in Ref. [2] where it was first proposed. One such refinement consists of specifying the integration contour in the degeneracy formula and noting that different contours can lead to different answers for the degeneracy [3]. The effect of varying the integration contours is in the form of discontinuous jumps in the degeneracy whenever the contour crosses a pole in the integration variable and picks up the corresponding residue. This has been interpreted as due to the decay of some 1/4 -BPS dyons into a pair of 1/2 -BPS dyons at curves of marginal stability, which are computed using the BPS mass formula.

Because for large charges, the decaying states are black holes and a mechanism is needed to explain exactly how they decay on curves of marginal stability. The answer turns out to be [4] that 1/4 -BPS black holes (for a given set of charges) exist both in single-centre and multi-centre varieties. For the latter, the separations of the centers are determined by the moduli [5]. If we specialize to two-centered dyons with both centers being 1/2 -BPS, then it was shown in Ref. [4] that as we approach a curve of marginal stability the two centers fly apart to infinity. On the other side of the curve the constraint equation has no solutions. This explains (in principle, though no method is known to explicitly count states of a two-centered black hole) the phenomenon of marginal stability and jumping in the counting formula, in terms of the disintegration of two-centered black holes. It should be noted that the degeneracy of single-centered black holes with the same charges does not vary across moduli space, therefore they exist either everywhere or nowhere.

We briefly review what is known about "rare" marginal decays in N = 4 string compactifications. Then we find precise form for the constraints on moduli space in order for such rare decays to take place. We examine and solve these constraints in a variety of special cases, to give a flavor of what they look like. Then using some known results on T-duality orbits, we will obtain the constraints in the general case [1]. Next we recursively identify the loci of marginal stability for multi-particle decays. Finally we examine the special-geometry formula for generic multi-centered black holes and write it in a form that relates their separations to curves of marginal stability for $n \geq 2$-body decays.

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Investigation of Calcium Chloride Aqueous Solutions/Hexane Interfaces: A Molecular Dynamics Study

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We have used molecular dynamics simulation to investigate hydrophilic/hydrophobic interfaces between calcium chloride aqueous solutions and normal hexane. The experimental and simulation results demonstrate the increasing impact of salt concentration on the liquid/liquid interfacial tension, hence negative adsorption of calcium chloride according to Gibbs addsorption isotherm. Moreover, we calculated the density profiles of hexane, water and the counter ions. The results reveal an electrical double layer near the interface and the less affinity of calcium cations towards the interface than that of chloride anions. Orientation of water molecules results in developing a positively charged interface and, consequently, accumiliation of anions close to charged interface. Our calculations show that the interfacial width decreases by increasing salt concentration. Therefore, consistent with calculated interfacial tension data, aqueous salt solutions are less miscible in normal hexane at higher salt concentrations. Figure 1 shows a typical view of our simulation box, containing water, n-hexane, and salt constituents.

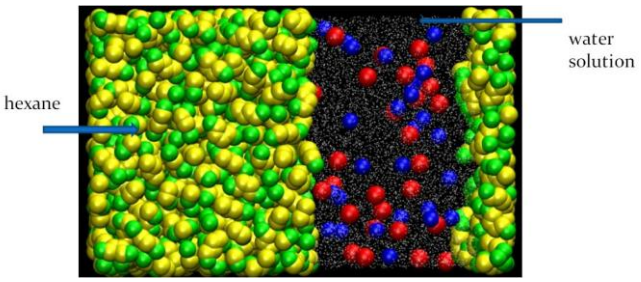

Figure 1: A typical molecular dynamics simulation box.

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A Discrete Stochastic Model for Pitting Corrosion

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Partial differential equations are generally resorted to for describing spatio-temporal (a)biological processes. Unfortunately, for most partial differential equations only approximate solutions can be found. Furthermore, they make abstraction of spatially explicit relations by assuming mean-field approximations, while their relative simplicity can be largely attributed to the simplifying assumptions under which they were derived. Of course, these shortcomings limit their usefulness for describing real-world phenomena. For these reasons other model types are increasingly explored, further stimulated by the growth of computational power during the last decades. Among these model types, the most promising are cellular automata (CAs) [1]. A CA is a spatio-temporal model based upon a discretized time, space and state domain, while its dynamics are governed by simple, spatially explicit rules. Despite this intrinsic simplicity, CAs are able to evolve complex spatio-temporal patterns. One of the fields where attempts are being made to employ CA-based models is in the field of corrosion [2].

Although many different aspects that influence corrosion, such as film formation, pH, differences in potential and heterogeneous composition of alloys, are being explored and are incorporated into models found in literature, most of them only establish a qualitative resemblance between the simulated model output and the real-world phenomenon, ignoring the importance of a sound model validation that is a prerequisite to have a model with predictive value. Only very recently, a few authors attempted to validate their CA-based model using time series of data, but with modest success. Furthermore, CA-based models in literature are usually two-dimensional, making them unsuited to model the growth of corrosion pits in the direction of the pit depth and surface simultaneously.

We have developed a 3D stochastic CA-based model that describes pitting corrosion and contains five model parameters that regulate the diffusion of the corrosive agent in the solution in which the metal is submerged, the pit initiation and pit propagation. In a first step, a sensitivity analysis of the model parameters is performed to study the importance of the different parameters as well as to optimize the design of the search grid for subsequent parameter optimization. Experimental time series of the number of pits, the affected metal surface area and the average depth of the pits for different concentrations of corrosive agent in the solution are available. These time series are used to parameterize the model and to study the effect of the concentration of the corrosive agent on the parameter estimation. This information can thereafter be used to perform model predictions.

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Nonequilibrium Green's function approach to simulations of active photonic nanostructures

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A reliable simulation of photonic devices requires good understanding of numerous physical aspects. The analyzed device can be considered as an inhomogeneous system of carriers, that interact with themselves, the lattice and the optical field. While in some situations, the quantum properties of the carriers play 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, see for example [1], [2]. 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 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 photonic 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 quantified. The description of such carrier-photon system in principle is described by the many-particle Schroedinger equation.

In the present work we summarize the applications of nonequilibrium Green's function (NEGF) approach to simulations of photonic nanostructures, with the emphasis on active devices [3]. We provide theoretical foundations of simulations of those devices where four types of quasi-particles (electrons, holes, phonons and photons) play an important role in the underlying physics. In this work we do not consider other types of quasi-particles, like excitons or plasmons.

General equations for photon Green's functions and polarizations will be established as well as their coupling to electron Green's functions through self-energies. Series of approximations are done to photon Green's function to allow for efficient numerical approach. All equations will be written in the non-orthogonal basis suitable for numerical calculations. As an example, the theory will be applied to analyze $Al_{0.2}Ga_{0.8}As/GaAs$ quantum well laser with the effective mass Hamiltonian. Major laser characteristics such as material and modal gain, threshold parameters, carrier and current densities are determined.

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Applications of Dynamical Systems and Differential Equations (CS-DSDE)

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Dynamics of a modified Leslie-Gower predator-prey model with Crowley-Martin functional responses and stochastic perturbations

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Interactions between populations and interactions of the populations with their environment has long been and will continue to be one of the dominant themes in both ecology and mathematical ecology due to its universal existence and importance (see [2]). Therefore mathematical models are important tools that can be used to understand aspects of various processes and to make predictions. In the paper [1], we have proposed and studied the predator-prey model with modified Leslie-Gower and Crowley-Martin functional responses under deterministic environment. We showed that the predator-prey model with Crowley-Martin functional responses has much richer boundary dynamics which includes the possibilities of extinction, permanence, stable or unstable equilibria and limit cycle. These results have important biological implications and indicate different results of the interaction of the predator-prey system.

In fact, population system are often subjet to environmental noise, i.e., due to environmental fluctuations (e.g. variation in intensity of sunlight, temperature, water level, etc.), parameters involved in models are not absolute constants, and they may fluctuate around some average values. Hence stochastic models provide some additional degree of realism compared to their deterministic counterpart. Based on these factors, stochastic population models have received more and more attention.
Therefore, it is interesting and important to consider and study a predator-prey model which incorporates a modified version of the Leslie-Gower with Crowley-Martin functional response and stochastic perturbations

$$\begin{cases} du(t) = u(t)\left(1-u(t)-\dfrac{v(t)}{(1+Au(t)+Bv(t)+ABu(t)v(t))}\right)dt+\alpha u(t)dB_1(t), \\ dv(t) = Cv(t)\left(1-\dfrac{Dv(t)}{u(t)+E}\right)dt+\beta v(t)dB_2(t), \end{cases} \tag{1}$$

where $u(t)$ and $v(t)$ represent the population densities at time t; $B_i(t)$, $i=1,2$ are independant brownian motions and $a_1, a_2, b, c, d, e, f, K, \alpha$ and β are model parameters assuming only positive values.

In this paper, we show the global existence of positive unique solution of the stochastic model (1), this is essential in any population dynamics model. That is, the solution of the system (1) is positive and not to explode in a finite time. And we show some asymptotic properties of the stochastic system (1). Morever, under some sufficient conditions, we conclude that the stochastic model is stochastically persistent in mean and extinct.

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Chaotic flow in single phase natural circulation loops

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In this paper the chaotic oscillations concerning the modeling of a general single phase-flow natural circulation loop are presented. By using a Fourier series expansion of appropriate variables, the conservation equations of mass, momentum, and energy have been modified to Lorenz system of equations. System stability is analyzed by linear theory and critical value for Rayleigh number has been determined. The results show that chaotic oscillations and strange attractor can appear in system by choosing a supercritical value for Rayleigh number.

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Hybrid Fixed Point Theorem For Abstract Measure Delay Integro-Differential Equations

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In this paper, an existence theorem for nonlinear abstract measure delay integro-differential equation is proved via hybrid fixed point theorems of Dhage under the mixed generalised lipschitz and caratheodory conditions the nonlinear alternative of Leray-Schauder type. An existence result of the extremal solution is also proved under certain monotonicity conditions using hybrid fixed point theorem on ordered Banach spaces. This contains Caratheodory as well as discontinuous cases of the nonlinearities involved in the equations. The abstract measure integro-differential equations in which ordinary derivative is replaced by the derivative of set functions namely the Radon-Nokodym derivative of a measure with respect to another measure. The above mentioned papers also include some already known abstract measure differential equations those considered in Sharma, Dhage and Ballale. Our existence results include the results of Sharma, Shendge and Joshi, Dhage and Bellale as a special case under weaker continuity condition.

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FEEDBACK STABILIZATION OF IMPULSIVE UNDERACTUATED MECHANICAL SYSTEMS BY USING LYAPUNOV CONSTRAINTS

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Impulsive underactuated mechanical systems is a class of underactuated mechanical systems constrained by kinematic constraints (holonomic, nonholonomic,...) which induce a discontinuous jumps on its velocities. The stability of such systems poses a great challenges due to the underactuation and to the dynamic change.

In this work we investigate on the feedback stabilization by using Lyapunov constraints that was founded by Grillo et al Ref[1] . The system evolves by two dynamics one before the impulsive effect and the second is after, the model is written in the Lagrangian framework Ref[2] . We impose to the two dynamics an affine kinematic constraints that is Lyapunov constraints, which is equivalent to the asymptotic stability conditions. As a result we prove that the necessary and sufficient conditions for the existence and uniqueness of control law leads to a system of partial differential equations whose solution is the required Lyapunov function, that should be unique and verify the impulsive effect condition.

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Control of the Landau–Lifshitz Equation

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The Landau–Lifshitz equation,

$$\frac{\partial \mathbf{m}}{\partial t} = \mathbf{m} \times \mathbf{m}_{xx} - \nu \mathbf{m} \times (\mathbf{m} \times \mathbf{m}_{xx}), \tag{1}$$

describes the behaviour of magnetization, $\mathbf{m}(x,t) \in \mathbb{R}^3$, inside a magnetic object. An example of such a magnetic object is a nanowire [1]. The subscript notation denotes

$$\mathbf{m}_{xx} = \left(m_1''(x,t), m_2''(x,t), m_3''(x,t)\right)$$

where the prime represents differentiation with respect to x. The cross product in equation (1) causes nonlinearity, hence making the system difficult to control. Control is further complicated by the presence of hysteresis in magnetization.

It is known [2] that the Landau-Lifshitz equation has an infinite number of stable equilibrium points. A control is desired which moves the system from one equilibrium to another, essentially controlling the behaviour of hysteresis and magnetization. An example of a physical control is an applied magnetic field, such as a nanowire subjected to an external magnetic field [1] which is a mechanism found in nano devices.

The purpose of the control is two–fold: (i) the control causes the initial equilibrium of (1) to no longer be an equilibrium of the controlled system, and (ii) the control ensures the second equilibrium is an asymptotically stable equilibrium point of the controlled system. The former is a simple consequence of adding the control term to (1). The latter is achieved by establishing the existence of a Lyapunov function.

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Replicator dynamics vs. agent-based models of Axelrod's norms game

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We create pure strategy versions of Robert Axelrod's well known norms and metanorms games. To analyze the evolutionary behaviour of these games, we utilize replicator dynamics complemented with agent based model simulations. Our

ndings show that the only evolutionarily stable strategy in the norms game is one in which a player defects and is lenient. This result is derived using classic game theoretical tools, and we conclude that Axelrod's original statement that the norms game always collapses holds. The metanorms game, however, has two evolutionarily stable strategies. The

rst is a repeat from the norms game, that is, a player defects and is always lenient. The other is one in which a player follows the norm and punishes those who are lenient and those who defect. We also shed light on what initial conditions will lead the population of players to certain evolutionarily stable states.

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A new multi-stage spectral relaxation method for solving chaotic initial value systems

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We present a new pseudo-spectral method application for solving nonlinear initial value problems (IVPs) with chaotic properties. The proposed method, called multi-stage spectral relaxation method (MSRM) is based on a novel technique of extending Gauss-Seidel type relaxation ideas to systems of nonlinear differential equation and using Chebyshev pseudo-spectral methods to solve the resulting system on a sequence of multiple intervals. In this new application the MSRM is used to solve famous chaotic systems such as the such as Lorenz, Chen, Liu, Rikitake, Rössler, Genesio-Tesi and Arneodo-Coullet chaotic systems. The accuracy and validity of the proposed method is tested against Runge-Kutta and Adams-Bashforth-Moulton based methods. The numerical results indicate that the MSRM is an accurate, efficient and reliable method for solving very complex IVPs with chaotic behaviour.

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Spectral approach in a 2D variational formulation for swirling flows in ducts with variable radius

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In [1] a new method for computing columnar swirling flows (with vanishing radial velocity) was developed using a variational formulation and Fourier-Bessel series approximations for both the streamfunction and the axial velocity profile. The inviscid separation zone as developed when the vortex breakdown occurs was captured using a simplified model corresponding to steady, axisymmetric, incompressible and inviscid swirling flow.

In this paper, we extend this approach in order to include also the radial velocity component and a variable cross section. We modify the functional in order to account for variable wall radius, as well as the flow evolution in the axial direction. The dimensionless flow force can be written

$$F(\psi, y_s) = \int_0^L \int_0^{y_w} (x)(\frac{v_m^2}{2} - \frac{c^2(\psi)}{2y} + h(\psi)), \tag{1}$$

with $v_m^2 == v_x^2 + v_y^2$ the mean velocity, v_x the axial component of the velocity and v_y the radial one, c- the circulation, h is the specific energy, ψ represents the streamfunction, y_w the radial extent of the cross-section at runner outlet.

In order to solve the resulting constrained variational problem for the streamfunction a Fourier-Bessel representation of the axial profile at the runner outlet was consider. The numerical algorithm for the 2D case will include the radial velocity as well. The results of the integration in the radial direction can be analytically provided and for the axial direction a finite difference scheme is used providing also the coupling between the cross-sections trough the variable radius duct. The obtained velocity profiles are compared to the ones of the numerical simulation providing an acceptable agreement.

Then we formulate a conclusion on the use of a 2D axi-symmetric model instead of the full 3D flow simulation, with huge savings in both computing time and resources.

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Analytical Integration of the Osculating Lagrange Planetary Equations in the Elliptic Orbital Motion

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In the field of orbital motion perturbation methods, a half century of works has produced a lot of analytical theories. These theories are either based on Hamiltonian developments and series expansions of the perturbing functions (Von-Zeipel, Brouwer, Lie-Deprit), or use iterative approximation algorithms (Kozai, Kaula). The differential system of the Lagrange planetary equations has also been solved using Cook's algorithm. Generally speaking, analytical theories have difficulties to deal with high eccentric satellite orbits, due to series expansions or due to the large number of terms in closed forms. The present work comes back to the original Lagrange planetary equations. One more time, the restricted three-body problem for an high eccentric satellite orbit is solved. It is a simple method intellectually efficient to analyse each effect of the Sun and of the Moon over one orbital period. Moreover, a long duration simulation allows to observe the secular effects on the orbital parameters. The goal of this paper is to solve the restricted three-body problem with a semi-analytical method accurate enough to deal with any high eccentric satellite orbit around an oblateness central body and perturbed by a third body. Osculating Lagrange planetary equations where the second members are the partial derivatives of simplified potentials of the Earth (J2), the Sun, the Moon and the direct Solar Radiation Pressure are solved in a quasi-inertial frame. Each numerical step of the algorithm provides the position of the third body thanks to Newcomb and Brown theories. First of all, the equations of the differential system are translated in osculating keplerian elements and the integration is formulated like in the Kozai's method [1]. Then each second member of each equation is integrated in a symbolic way with the software *Mathematica*, this is a major point. Another major point is the control of the constants of the elliptic characteristic functions of the integration. The semi-analytical algorithm and the equation of time are detailed. Finally, the results of the method for solar and lunar effects on a Geostationary Transfer Orbit, a High Elliptic Orbit and for an eccentric Mean Earth Orbit are provided. Each computation, as a non-optimized mock-up, leads to more precise qualitative results than precise ones. As a conclusion, the high eccentric satellite orbit has been solved in an analytical way, but also as educational.

Without symbolic calculator this work would have been very difficult, moreover it would not have been. For example a simple integral of the 62 computed integrals:

$$\int \frac{1}{(1+e\cos(v))^4}dv = \frac{1}{6}\left(\frac{(e\sin(v)(8e^4+(4e^2+11)e^2\cos(2v)+6(e^2+9)e\cos(v)+e^2+36))}{(2(e-1)^3(e+1)^3(e\cos(v)+1)^3)}\right.$$
$$\left. - \frac{6(3e^2+2)\tanh^{-1}\left(\frac{(e-1)\tan\left(\frac{v}{2}\right)}{\sqrt{e^2-1}}\right)}{(e^2-1)^{\frac{7}{2}}}\right) + constant$$

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Nutrient transport through heterogeneous soil medium

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Analytical solutions are obtained for conservative nutrient transport in a one-dimensional semi-infinite heterogeneous porous domain. The nutrient dispersion parameter is considered uniform while the seepage flow velocity is considered spatially or position dependent. Retardation factor is also considered and taken inversely proportional to square of the flow velocity. The seepage flow velocity is considered inversely proportional to the position or spatially dependent function. The solution is derived for two cases: former one is for uniform pulse type input point source and latter is for varying pulse type input point source. The second condition is considered at the far end of the medium. It is of second type (flux type) of homogeneous nature. In both cases initially domain is not nutrient free. Laplace Transform Technique is used to get the analytical solutions of the present problem. In the process a new space variable is introduced. The solutions are graphically illustrated. The effects of heterogeneity of the medium, on the nutrient transport behaviour, in the presence of the source and in the absence of the source, are also studied.

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Collision properties of solitary waves for the Gardner equation

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We study the physical and collision properties of the combined KdV-mKdV solitons given by the Gardner equation which posses a single soliton solution characterized by a *sech* profile with a speed $c > -3/2$ and a constant frequency. We make a physical form of the 2-soliton solution where the fast soliton moves with speed c_1 and the slow soliton moves with speed c_2. In the collision described by the 2-soliton solution, the solitary waves preserve their shapes and speeds, but undergo a shift in position where the fast soliton overtakes the slow soliton if their speeds have same direction, and two solitons cross head-on if the speeds have opposite direction. For a collision there exists three different types of interaction (bounce-exchange, merge-split, absorb-emit) which depend on the relative ratio of speeds c_1/c_2 and the relative orientation of the two solitary waves.

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Stability in a distributed delay differential equation

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The subject of the talk is the asymptotic stability analysis of the trivial equilibrium of a scalar and linear delay differential equation with two (infinite) distributed delays characterised by general delay kernels, and given by

$$x'(t) = -x(t) + \alpha \int_0^\infty x(t-\tau) g_\alpha(\tau) d\tau + \beta \int_0^\infty x(t-\tau) g_\beta(\tau) d\tau \,, \tag{1}$$

where $\tau \in \mathbb{R}^+$ is a distributed delay, $\alpha, \beta \in \mathbb{R}$, and g_α, g_β are general time-delay kernels. Such equations occur as the linearisation about an equilibrium point for models with two feedback loops. The delay kernels are non-negative bounded functions defined on $[0,\infty)$. Assuming that the presence of distributed delay does not affect the equilibrium values, we normalise the kernels so that

$$\int_0^\infty g_\alpha(s) ds = 1 = \int_0^\infty g_\beta(s) ds \,. \tag{2}$$

The characteristic equation of (1) at the trivial equilibrium $x^* = 0$ is given by

$$D(\lambda) = \lambda + 1 - \alpha \int_0^\infty e^{-\lambda\tau} g_\alpha(\tau) d\tau - \beta \int_0^\infty e^{-\lambda\tau} g_\beta(\tau) d\tau = 0 \,, \tag{3}$$

where $\lambda \in \mathbb{C}$ is the characteristic exponent. The continuous extension at $\lambda = 0$ is $D(0) = 1 - \alpha - \beta$. In this presentation, we shall develop a variety of results to characterise the stability region of (1) in the (α, β)-parameter space. The results are based on the exact analysis of the characteristic equation (3) of the delay differential equation (1).

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Stability Analysis of a Human-Phlebotomus Papatasi-Rodent Epidemic Model

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Cutaneous leishmaniasis, also called Biskra button, represents a serious public health problem in Algeria. In the aim to understand the transmission dynamics of cutaneous leishmaniasis in the human-Phlebotomus papatasi-rodent cycle, and to improve the preventive strategies set up in Algeria, we developed a deterministic model. The model includes an incidental host for human which acts only as a sink of infection, a primary reservoir host for rodent which acts as a source and a sink of infection, and a secondary reservoir host for Phlebotomus papatasi which have a role in transmission by acting as the liaison between incidental host and primary reservoir. The global stability of the equilibria of the proposed model shows that the threshold conditions for disease persistence, are completely determined by the reproduction number, and do not explicitly include parameters relating to the dynamic transmission in the incidental hosts, which means that the disease becomes endemic if it persists endemically in the primary reservoir hosts, and therefore the control measures should be directed towards reservoir hosts. This is illustrated via numerical simulations of the model using parameters generated from data from Biskra-Algeria.

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Scattering states of a particle, with position-dependent mass, in semiconductor double heterojunction

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Treating particles with position dependent effective mass (PDEM) because of varying doping concentration in semiconductor devices of extremely small dimensions, is found to give better explanation to observed phenomena. Such formalism is extremely important in describing the electronic and transport properties of quantum wells and quantum dots, impurities in crystals, He-clusters, quantum liquids, semiconductor heterostructures, etc. If a sufficiently thin layer of a narrower (wider) bandgap material is sandwiched between two layers of a wider (narrower) bandgap material, they form a double heterojunction, called a single quantum well (barrier).

On the other hand, PT symmetric waveguides fabricated from iron-doped $LiNbO_3$ are now a reality. Such non Hermitian quantum systems with space-time (PT) symmetry, show peculiar properties unknown to Hermitian ones — e.g., real and discrete spectrum under certain conditions, violation of Fresnel's Law of Bragg scattering, double refraction, power oscillations, non-reciprocal diffraction, handedness or left-right asymmetry, anomalous transport, unidirectional invisibility, etc. Additionally, they admit exceptional points (EP) in the discrete spectrum, when real energy switches to complex conjugate pair, and spectral singularities (SS) in the continuous spectrum, where reflection and transmission coefficients blow up, etc.

We shall present exact analytical results for the scattering states of a particle with PDEM, inside a single quantum well/barrier, for Hermitian and non Hermitian potentials. Exact analytical results are important for conceptual understanding of physics, providing a valuable platform for checking and improving approximate models and numerical results, in various areas of material science and condensed matter. In particular, we consider the model

$$\begin{array}{lcll} V & = & V_R(z)+iV_I(z)\,, & m=m(z) \quad , \quad a_1<z<a_2 \\ V & = & V_{01}=V_R(a_1)\,, & m=m_1=m(a_1)\,, \quad -\infty<z<a_1 \\ V & = & V_{02}=V_R(a_2)\,, & m=m_2=m(a_2)\,, \quad a_2<z<\infty \end{array} \tag{1}$$

where a_1 and a_2 represent the heterojunctions. For Hermitian systems, $V_I(z)=0$.

We observe that for both Hermitian and non Hermitian cases, PDEM introduces a non linear component in the otherwise plane wave solutions. The reflection and transmission amplitudes, R and T respectively, are observed to display a characteristic behaviour — with increasing energy, $|T|^2$ increases, finally reaching unity, whereas $|R|^2$ follows the reverse trend and goes to zero. In case of non Hermitian PT symmetric quantum systems, it is observed that at least two of the general features of such potentials — viz., left-right asymmetry and blowing up of $|R|$ and $|T|$ at SS — are preserved even for particles with PDEM. The findings are plotted in a series of graphs.

This simple model gives an insight into the basic physics of the electronic properties of a double heterojunction semiconductor device with PDEM. Actual materials require a more rigorous approach, to be taken up shortly.

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Retention of Eventual Stability of Invariant Sets of Impulsive Differential Systems

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ABSTRACT: Consideration is given to a system of differential equation with impulsive action at fixed time instants and perturbed right hand sides[7]. In [1] and [2], criteria have been obtained for retention of uniform asymptotic stability of invariant set of impulsive differntial sytems, under vanishing perurbations. In [3], [4], [5] and [6], the notion of eventual stability has been introduced for impulsive systems of differential equations and results for uniform eventual stability , asymptotic eventual stability have been given for perturbed and non perturbed systems. In our paper, the work of R.I. Gladilina and A.O. Ignat'ev[1] and [2] has been extended and criteria for retention of eventual stability of invariant set of a non linear system of impulsive differential equations with impulse action at fixed time instants have been obtained by using piecewise continuous Lyapunov functions. It is assumed that the system has an invariant set M. Two theorems have been proved. An example is also given to support the theoretical result.

Keywords: Invariant Sets, Eventual stability, Piecewise continuous Lyapunov Functions.

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Equivalence of the MTS Method and CMR Method for Delay Differential Equations

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It is important to compute normal forms of differential equations in the study of nonlinear dynamical systems, which is particularly difficult and tedious for higher-dimensional and higher-order systems. The center manifold reduction (CMR) [1] and multiple time scales (MTS, or simply multiple scales (MS)) [2] are two useful techniques for computing the normal forms of differential equations. For differential systems involving time delays, the computation of normal forms is more complicated and time consuming, compared to that of ordinary differential equations. For delay differential equations (DDEs), the CMR method is usually applied to compute normal forms [3]. Recently, the MTS method has also been directly applied to DDEs for computing normal forms and shown to be simpler than the CMR method [4, 5, 6, 7]. In order to show the equivalence of the two methods, researchers usually apply the two methods to a particular system to obtain two sets of normal forms, and then compare them. If they are identical, then the two methods are proved to be equivalent. This is not only time consuming, but also easy to make mistakes.

In this talk, we will show the equivalence of the MTS method and the CMR method in computing the normal forms of DDEs. The equations considered include general delay differential equations (DDE), neutral functional differential equations (NFDE) (or neutral delay differential equations (NDDE)), and partial functional differential equations (PFDE). The delays involved in these equations can be discrete or distributed. Particular attention is focused on dynamics associated with the semisimple singularity, and both the MTS and CMR methods are applied to compute the normal forms near the semisimple singular point. The two methods are proved to be equivalent in computing the normal forms of these differential equations with delays, at least up to a reasonable order which is enough in real applications. It is shown that the computation of using the MTS method is simpler than that of the CMR method. Different types of practical examples with delays are presented to demonstrate the application of the theoretical results, associated with Hopf [5], Hopf-zero [6], and double-Hopf [7] singularities.

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Pricing and Hedging Index Options with a Dominant Constituent Stock

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In this paper, we examine the pricing and hedging of an index option where one constituent stock plays an overly dominant role in the index. Under a Geometric Brownian Motion assumption we compare the distribution of the relative value of the index if the dominant stock is modeled separately from the rest of the index (see Eq. 1), or not (see Eq. 2). The former is equivalent to the relative index value being distributed as the sum of two lognormal random variables

$$Y = c_1 e^{Z_1} + c_2 e^{Z_2}, \text{ where } Z_i \sim \mathcal{N}(\mu_i, \sigma_i), \ i = 1,2 \tag{1}$$

and the latter is distributed as a single lognormal random variable

$$X = c_3 e^{Z_3}, \text{ where } Z_i \sim \mathcal{N}(\mu_i, \sigma_i), \ i = 3. \tag{2}$$

Since $X \neq Y$ in distribution, with Y having fatter tails, we compare the two models. The validity of this theoretical result is verified against empirical stock market data. We look at two main models representing these cases: first, we use numerical methods to solve the two dimensional problem directly (see Eq. 3); second, we make simplifying assumptions (see Eq. 4) to reduce the two dimensional Black-Scholes problem to a one dimensional Black-Scholes problem that can be solved analytically (see Eq. 5). The two dimensional PDE for V(A,B,t) is

$$V_t + \frac{1}{2}\sigma_A^2 A^2 V_{AA} + \rho\sigma_A\sigma_B AB V_{AB} + \frac{1}{2}\sigma_B^2 B^2 V_{BB} + rAV_A + rBV_B - rV = 0 \tag{3}$$

with the terminal condition $V(A,B,T) = (K - A + B)^+$, where A is the dominant stock and B is the rest of the index. So our simplifying assumption is that

$$V_{AA} = V_{AB} = V_{BB} = V_{II} \text{ and } V_A = V_B = V_I \tag{4}$$

from $I = A + B$, so we let $\alpha = \frac{A}{A+B}$ to reduce the full PDE (see Eq. 3) to the one dimentional PDE for V(I,t)

$$V_t + \frac{1}{2}(\sigma^*)^2 V_{II} + rIV_I - rV = 0 \text{ where } (\sigma^*)^2 = \sigma_A^2\alpha^2 + 2\rho\sigma_A\sigma_B\alpha(1-\alpha) + \sigma_B^2(1-\alpha)^2 \tag{5}$$

with terminal condition $V(I,T) = (K - I)^+$.

Since the terminal conditions are non-smooth the numerical methods are verified by comparison with a related Margrabe exchange option, a two dimensional option with a true analytic solution.

Attributes of the models that we compare are the relative option price differences, expected hedging profits, and computation time and complexity. For different levels of α, one model will be superior to the other and we will make recommendations for when to use each model for effective and accurate pricing and hedging.

This work is significant in options trading because when a stock becomes dominant in its index the distribution of the returns changes. Even if the effect is small, given the millions of dollars exposed to index option trades, it has a material impact.

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Weather Derivatives with Applications to Canadian Data

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We applied two daily average temperature models to Canadian cities data and derived their derivative pricing applications. The first model is characterized by mean-reverting Ornstein-Uhlenbeck process driven by general Lévy process with seasonal mean and volatility. As an extension to the first model, Continuous Autoregressive (CAR) model driven by Lévy process is also considered and calibrated to Canadian data. It is empirically proved that the proposed dynamics fitted Calgary and Toronto temperature data successfully. These models are also applied to derivation of an explicit price of CAT futures, and numerical prices of CDD and HDD futures using fast Fourier transform. The novelty of this paper lies in the applications of daily average temperature models to Canadian cities data and CAR model driven by Lévy process, futures pricing of CDD and HDD indices.

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Fast pricing of discretely monitored exotic options using the Spitzer identity and Wiener-Hopf factorization

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The application of transform techniques to price derivative contracts is rather recent. One of the first and most important contribution is probably the article by Carr and Madan [1], where the authors show how to price European options exploiting the fast Fourier transform. Similar techniques were developed later for path-dependent derivatives [2, 3, 4]. Here we present fast and accurate algorithms based on the Spitzer identity and the Wiener-Hopf factorization to price barrier, lookback (or hindight), and quantile options when the underlying asset evolves as an exponential Lévy process and the monitoring is done at discrete time intervals.

Our fast numerical methods have a computational cost independent on the number of monitoring dates, thanks to the z-transform approach combined with the Euler summation [5, 6]. The error decays exponentially with respect to the number of discretization points, except for double-barrier options, where the decaying is quadratic, thanks to computing the required factorizations or decompositions functions with a numerical implementation of the Hilbert transform based on fast Fourier transforms and sinc functions [7]. The proposed algorithms are based on the Spitzer identity [8], an important result regarding the distribution of the discrete extrema for a process with independent and identically distributed increments, like the considered Lévy processes. Spitzer provides a closed formula for the z-transform of the characteristic function of the extrema on a grid. Even if the Spitzer identity has already been used in option pricing [3, 9, 10], according to our knowledge this is the first work where its application and its efficient numerical implementation to a general Lévy process is presented.

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Valuation of the Peterborough Prison Bond

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Social Impact Bonds (SIBs) are an innovative financing vehicle that aims to mobilize private capital for social programs. Private and philanthropic investors pay for preventive social interventions, which have the potential to save government money on its future expenditures, and if certain social outcomes are achieved part of the government's savings is paid to the SIB investors. As a result, investors earn a blended social and financial return that is uncorrelated with the financial market; government reduces its risk of spending tax-payers money on unsuccessful projects; social service providers get the needed cash upfront; and the society at large benefits as overall quality of life improves.

The first SIB was issued in the UK in 2010 to reduce recidivism among adult male prisoners serving short term sentences in the Peterborough Prison (see Ref. [1]). It raised £5 million of investment funding to provide rehabilitation services to three cohorts of 1000 prisoners each. Payouts will be proportional to the reconviction rate if the rate drops by at least 10% for a single cohort, or by 7.5% for all three cohorts combined, and with a cap on the total payout.

Most of the literature on the SIBs so far has been focused on the opportunities, challenges, and the related policy issues (see Ref. [1,2]), and little effort has been made to provide a mathematical framework to determine a fair price for such instruments. However, for SIBs to become a publicly traded security, such a framework is necessary to allow investors to compare its risk and return characteristics with other securities. Here, we aim to provide such a pricing framework.

We rely on the incomplete market pricing methodologies as the underlying risky asset (recidivism rate) is not traded, and the SIB cannot be hedged perfectly. We choose indifference pricing and the Wang transfrom (see Ref. [3]) as pricing methodologies. A model for the recidivism rate of the Peterborough Prison cohorts is obtained by fitting the skew normal and the beta distributions to a weighted histogram of the outcomes of past prison rehabilitation programs, while adjusting for the differences between these programs. The fair value of the bond is then determined by adjusting for both the risk present in the bond's payout, and the ambiguity associated with the mathematical model for the underlying reconviction rate. Sensitivity of the bond price to the relevant parameters is discussed. Effect of the social impact of the bond on the fair price is also studied from the perspective of a socially responsible investor – one who would be willing to trade off financial return for social impact. Results suggest that indifference pricing with the skew-normal distribution is the most flexible pricing mechanism, and that the bond is a high risk, high yield instrument, with the ambiguity in the model for the reconviction rate being the most significant source of uncertainty.

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Basket Option Pricing with Lévy Processes using the Mellin Transform

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The shortest path between two truths in the real domain passes through the complex domain. -Jacques Hadamard

An option is a financial security that presents its holder with the right, not the obligation, to purchase a given amount of an underlying asset at some future date. With global issuance of 24.9 billion contracts annually, proper valuation is a significant concern among institutional, governmental, and personal traders who use options to invest or mitigate risk by hedging. The objective of option pricing theory is to obtain models that accurately portray empirical features of option prices while subject to general assumptions that govern financial markets.

Since Black and Scholes seminal paper in 1973, the study of option pricing has invoked tremendous academic and industrial interest [1]. However, the Black-Scholes framework requires certain improvements, since it fails to account for non-constant volatility and the empirical observation that log-returns of assets are not normally distributed, but instead exhibit significant skewness, kurtosis, and bear the ability to change discontinuously. This led to the representation of stochastic volatility as a Lévy process; a random process with independent, stationary, and stochastically continuous increments [2]. Due to their general construct and obedience of observed regularities, we choose to study option pricing models governed by Lévy processes.

Following recent methods introduced by Panini and Srivastav, we employ the Mellin transform as a tool for obtaining analytical solutions to the option valuation problem [3]. For a function $f(x) \in \mathscr{R}^+$, the Mellin transform is defined as the complex function,

$$\mathscr{M}\{f(x);s\} = f^*(s) = \int_0^\infty f(x)x^{s-1}dx \tag{1}$$

where $s \in \mathscr{C}$ is defined on a vertical strip of analyticity in the complex domain. Using this integral transform, closed-form solutions have been obtained for Asian, European, European Power, European Basket (for $n = 2$ underlying assets), and European options driven by Lévy processes. Analytical approximations exist for American options with and without assets driven by a Lévy process, however no closed-form solutions exist (by any method).

By harnessing the Mellin transform, we obtain analytical approximations to European and American options with n underlying assets (i.e. basket options) driven by Lévy processes. As a corollary, we generalize previous results by providing solutions for non-Lévy-driven $n > 2$ European and American basket options. For all cases, numerically fast solutions are presented by exploiting the relationship between the Mellin and Fourier transform. Using these formulas, we compute implied option prices for historical foreign exchange rates of major currencies.

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Investigating the Market Price of Volatility Risk for Options in a Regime-Switching Market

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Previous investigations [1] have shown that a non-zero market price of risk is consistent with market data, by quantifying the relationship between implied and realized volatility. To bridge the gap between theoretical option pricing models and observed option prices, it is necessary to price the volatility risk inherent in financial markets. Assuming a random volatility process can be well modelled by shifts between high and low regimes, pricing equations for European options, $C^H(S,t)$ and $C^L(S,t)$, are derived where $C^H(S,t)$ (resp. $C^L(S,t)$) denotes the option price conditional on the stock price process being in a high (resp. low) volatility regime. The state-dependent market prices of volatility risk, $m_H(S,t)$ and $m_L(S,t)$, arise in our coupled pricing equations from the typical contract independence assumption.

$$\frac{\partial C^i}{\partial t}(S,t)+\frac{1}{2}\sigma_i^2 S^2\frac{\partial^2 C^i}{\partial S^2}(S,t)+rS\frac{\partial C^i}{\partial S}(S,t)-rC^i(S,t)+\Big(\lambda_j-m_i(S,t)\Big)\Big(C^j(S,t)-C^i(S,t)\Big)=0, \qquad (1)$$

where $i\in\{H,L\}$ and $i\neq j$.

For risk-neutral traders whose market price of risk is zero, our coupled system of equations reduces to Boyle and Draviam′s result [4]. Both directly from our pricing equations and building upon previous work by Mielkie and Davison [2] in which an approximate solution for equation (1) was derived, we analyse the impact of the market price of volatility risk on theoretical option prices. We prove that financially reasonable results are only obtained when the market price of volatility risk takes values restricted to a certain set. In particular, we show that negative state-dependent market prices of volatility risk are necessary in order for the option prices and corresponding hedge ratios to be financially rational. Our regime-switching option price solutions and their associated implied volatilities are explored through both limiting arguments and with numerical solutions. We conclude by discussing valuable intuition arising from this study.

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Utility Indifference Pricing: A Time Consistent Approach

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This paper considers the optimal portfolio selection problem in a dynamic multi-period stochastic framework with regime switching. The risk preference is of exponential (CARA) type with a time changing coefficient of risk aversion. The market model is incomplete and there are two risky assets: one tradable and one non-tradable. In this context the optimal investment strategies are time inconsistent. Consequently the subgame perfect equilibrium strategies are considered. The utility indifference ask price of a contingent claim written on the risky assets is computed via an indifference valuation algorithm. We examine the changes in the utility indifference ask price due to changes in model parameters.

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Parametric Estimation of Stationary Stochastic Processes under Indirect Observability

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Statistical estimation of parameters in the effective stochastic model given a discrete dataset is an important requirement in various scientific studies. However, a common pathological situation is the unobservability of the data. This means that the available data cannot be observed directly. Instead, observations of a suitable approximating process are available. Namely,

$$Y_t^\varepsilon = X_t + \varepsilon_t,$$

where Y_t^ε is the observed process and X_t is the true process.

One of the most striking examples is the realized volatility in financial market. Therefore, there may be an inherent difference between the data and the effective stochastic model which introduces additional errors in parameter estimators due to the unobservability.

In our work we consider the estimation of parameters for the volatility process in the stochastic Heston model when the volatility process is not observed. It is known that the volatility process can be approximated by the quadratic variation of the stock price. Our goal is to understand how these errors propagate into the parameter estimators in the equation for the volatility. Motivated by the Heston model, we develop a general theory of consistent parametric estimation. In particular, we introduce a consistent and robust estimator for the class of strong mixing stationary stochastic processes. We analyze the speed of convergence of estimators and develop an explicit criteria for the optimal sub-sampling scheme which minimizes the computational cost. Last, a successful application of our results is demonstrated by estimating the parameters of volatility process in Heston model with realized volatility.

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Robust Second-order least-squares estimation for regression with autocorrelated error: application of FMW and Generalized M-Estimates based methods

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In his recent paper, Wang and Leblanc [1] have shown that the second-order least squares estimator (SLSE) is more efficient than the ordinary least squares estimator (OLSE) when the errors are iid (independent and identically distributed) and the error distribution has a nonzero third moment. In Rosadi and Peiris [2], the theory of SLSE is applied for regression models with autocorrelated errors. Rosadi and Peiris [2] derived the the asymptotic normality property of the corresponding estimator and it is also provided a simulation study to compare the performance of SLSE, OLSE and Generalized Least Square estimator (GLSE). From Rosadi and Peiris [2] we can summarize the following results: from the simulation result, it shows that the SLSE performs well for estimating the parameters of the model and gives small bias. For less correlated data, the standard error (s.e.) of SLSE lies between s.e. of OLSE and GLSE, which can be interpreted that adding second moment information can improve the performance of the estimator. However, for more correlated data, the SLSE is becoming less robust than OLSE. The s.e. of GLSE are the smallest, which is consistent with the theoretical result (Gauss-Markov-Aitken theorem). In this paper, we consider a new method to robustify the SLSE in case of correlated data, and evaluate the performance of the robust method by the meaning of the simulation study. In our implementation, to increase efficiency of the estimators, we consider weight function as in Filzmoser, Maronna and Werner [3] (FMW method).To remove the effect of "bad leverage points" due to y-outlier, we apply the class of generalized M-estimates (GM-estimates) for the time series residuals (see e.g. Maronna, Martin and Yohai [4]). This result is the extension of the result presented in Rosadi [5].

Keyword: robust second-order least square, autocorrelated error, ordinary least square , generalized least square, asymptotic normality

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CVaR Robust Mean-CVaR Portfolio Optimization

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One of the most important problems faced by every investor is asset allocation. An investor during making investment decisions has to search for equilibrium between risk and returns. Risk and return are uncertain parameters in the suggested portfolio optimization models and should be estimated to solve the problem. The estimation might lead to large error in the final decision. One of the widely used and effective approaches for optimization with data uncertainty is robust optimization. In this paper, we present a new robust portfolio optimization technique for mean-$CVaR$ portfolio selection problem under the estimation risk in mean return. We additionally use $CVaR$ as risk measure, to measure the estimation risk in mean return. Moreover, to solve the model efficiently, we use the smoothing technique of Alexander et al. We compare the performance of the $CVaR$ robust mean-$CVaR$ model with robust mean-$CVaR$ models using interval and ellipsoidal uncertainty sets. It is observed that the $CVaR$ robust mean-$CVaR$ portfolios are more diversified. Moreover, we study the impact of the value of confidence level on the conservatism level of a portfolio and also on the value of the maximum expected return of the portfolio.

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Pricing exotic options under the time-changed Brownian motion model by variance reduction and quasi-Monte Carlo methods

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Empirical studies with worldwide financial data show that a special type of Lévy processes - the time-changed Brownian motion, can fit the real financial data better than the well-known Black-Scholes-Merton's model. The use of these more realistic and complex models for asset prices gives rise to many new and challenging problems for derivative pricing, hedging, portfolio optimization and risk management. For example, efficient numerical methods dealing with derivative pricing and risk management under Lévy models are in high demand due to the lack of closed formulas for options under Lévy models. The Monte Carlo simulation method is indispensable to deal with high dimensional problems so far. This method is widely used in many fields. Its main drawback is the slow convergence. To accelerate the convergence, variance reduction (VR) methods, effective dimension methods, quasi-Monte Carlo (QMC) methods and their combinations have been developed. The idea of VR is not new, but to design an efficient VR method is always challenging, especially for complex problems such as option pricing and hedging for asset prices under Lévy models. There is very limited literature on this topic.

In this paper, we consider the problem of exotic option pricing under the exponential time-changed Brownian motion model for the underlying asset price by variance reduction methods combined with quasi-Monte Carlo methods. In particular, the case of the lookback option is studied in more detail, where the lookback option under the Black-Scholes model for the asset prices, the geometric Asian option, as well as a random variate conditional on the geometric mean of asset prices are used as control variates. Initial numerical results with various model parameters and strike prices show that variances are reduced by both antithetic variate and control variate methods. The variance reduction ratios are significantly improved when quasi-Monte Carlo methods are combined. For example, the variance reduction ratio by control variate method is up to 2.73×10^5 for an at-the-money discrete fixed strike lookback option with 32 monitoring points.

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Simulation of Greeks of multiasset options under exponential subordinated Brownian motion models by Malliavin calculus and quasi-Monte Carlo methods

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The option sensitivities or Greeks are important in financial hedging and risk management. However, values of option Greeks are even harder to obtain than values of options themselves. It is difficult to deal with options with discontinuous payoff functions by the conventional finite central difference method. While the likelihood ratio method is helpless if the density functions do not exist or hard to find. A third approach - the Malliavin calculus method, was proposed about a decade ago and showed its advantages over the other two methods for exotic options. The main idea of this method is to express the Greeks in terms of option payoff functions multiplied by weight functions depending on Malliavin derivatives.

This paper discusses simulation of option Greeks for multi-asset options under the subordinated Brownian motion model by Malliavin calculus combined with Monte Carlo and quasi-Monte Carlo methods. By using the chain rule, integration by parts, the reflection principle, etc. from Malliavin calculus, as well as the tower property of conditional expectation, we are able to express Greeks in terms of the expectations of the option payoff functions multiplied by the weights involving Malliavin derivatives for multi-asset options in both path independent and path dependent cases. In the one asset case, the formulas recover those found in the literature. Numerical results show that the Malliavin calculus method is usually more efficient than the finite difference method for options with non-smooth payoffs. The superiority of the former over the latter is even more significant when combined with quasi-Monte Carlo methods. For example, when simulating Γ_{11} or Γ_{12} of a basket type down-and-out option or a corridor option, the efficiencies reach up to more than ten thousand times in a two-asset case and more than one thousand times in a six-asset case.

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American option pricing under time-changed Brownian motion models

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American options are widely used in financial investment. The problem of efficient pricing of (multi-asset) American options is always challenging. This is true even under the well-known Black-Scholes-Merton's model for the underlying asset prices due to the fact of lack of closed formulas for American option prices. The regression based method is a popular approach to deal with American option pricing problems in high dimensions. Its main drawbacks are: (1) it is hard to determine the number of basis functions used in regression in advance; and (2) it is difficult to estimate American option sensitivities or Greeks by this method. The Malliavin calculus approach has been proposed recently for pricing and hedging American options under the Black-Scholes-Merton's model for the underlying asset prices. With this method, option prices and Greeks, such as *Delta*s, are approximated by quantities involving ratios of unconditional expectations. In terms of computational speed, this method is not as fast as the regression method. But it can easily estimate the option Greeks while it is difficult for the other method to do so. In this paper, we consider the problem of multi-asset American option pricing under the exponential time-changed Brownian motion model for the underlying asset prices by regression based method, as well as Malliavin calculus method combined with variance reduction methods, localization method and quasi-Monte Carlo methods.

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Optimal Annuitization Timing With Stochastic Interest Rates

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Defined Benefit (DB) pension plans are vanishing in most of developed countries. The demise of DB Pensions forces more retirees to use defined contribution (DC) pension plan to hedge the longevity risk. The average life span has increased by more than 30 years during the 20th century in Canada. There maybe more than thirty years to live after individuals get retired. How to manage the nest egg in retirement so that retirees will have a decent living standard after retirement? Should retirees annuitize his nest egg? If yes, What's the optimal annuitization time? Will mortality rate and risk aversion affect the optimal annuitization time? The value from delaying annuitization is very valuable under an all-or-nothing framework. While in anywhere anytime framework, the utility-maximizing retiree should acquire a base amount of annuity income and then annuitize additional amounts (Milevsky and Young, 2006). Individuals can get welfare gains up to 40% of their financial wealth by adjusting portfolio allocation and purchasing variable annuities gradually over time (Horneff et al. 2008).

We study optimal annuitization under stochastic interest rates in an all-or-nothing framework. The risk-free rate is modeled by Cox-Ingersoll-Ross (CIR) process while mortality rate is assumed to be Gompertz. This is a free boundary problem similar to the American put option problem. We reformulate the free boundary problem as a linear complementarity (LCP) problem and solved it numerically using the projected successive over-relaxation (SOR) method. Numerical results will be presented based on realistic parameter values.

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A Monte Carlo Measure to Improve Fairness in Equity Analyst Evaluation

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For decades, research analysts have been supplying stock recommendations to clients. To help clients decide which of these analysts to listen to, numerous analyst ranking systems have emerged. Examples include The Wall Street Journal's "Best on the Street" annual awards, and the Starmine analyst performance measurement system. These systems are often variatations on a method we term the "portfolio method", whereby a hypothetical portfolio is formed with one long unit for each stock where the analyst makes a positive recommendation and one short unit for each negative recommendation. Analysts are then compared by the final value of their portfolios. Of the pitfalls to this method, one most troubling is that the analysts are generally covering different sets of stocks over different time periods. Thus, each analyst has access to different opportunites and just comparing portfolio values is unfair. In response, we present a Monte Carlo method where, for each analyst, we generate numerous "pseudo-analysts" with the same coverage over the same time periods as the real analyst. For each one of our generated pseudo-analysts, we sample from the distribution of all real analyst recommendations both for recommendation length and direction (i.e. positive, neutral, negative). In essence, we are able to compute how well the analyst performs against simple random selection by finding the percentage of pseudo-analysts s/he outperforms. Using this output, we are better able to compare analysts, adjusted for their individual opportunities. We draw comparisons between our results and the results from the existing systems, showing why those systems are less precise in reflecting analyst performance.

Computational Mechanics and Engineering (CS-MECHE)

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Stochastic modeling of the Oil Sands operations under environmental constraints

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The Alberta's Oil Sands represent the third largest proven oil reserves in the world. Part of the world future energy security depends on the expansion and further development of this industry. The operations of the Oil Sands is subject to a number of uncertain parameters for economic growth in the long-term outlook. The main uncertainties posed over the Oil Sands sector are related to the price of primary fuels, operational enhancements and environmental restrictions. In this work, the deterministic energy optimization model for the Oil Sands operations proposed by Betancourt-Torcat et al. [1] has been extended to account for uncertainty in the natural gas price and Steam-to-Oil ratio (SOR). The new extended model includes Green HouseGas (GHG) emissions and freshwater withdrawal allowance constraints. The problem was formulated in the General Algebraic Modeling System (GAMS) as a stochastic MINLP.

The application of the stochastic energy optimization model for the Oil Sands includes results reflecting the uncertain outcomes and enabling optimal arrangement of the energy supplier and oil producer infrastructures at minimum energy costs. In the present work, the model's capabilities are shown using two case studies considering uncertainty whereas the deterministic case is presented as reference for comparison purposes. The case studies examined under uncertainty consider the forecasted oil production scenario for the year 2035 in an uncertain environment, where the price of natural gas is volatile (e.g., fuel price) and the SOR (e.g., operational factor) unknown. The results of the stochastic model were compared with those of the deterministic model by examined the expected values of the stochastic approach and those of the deterministic solution. The results presented in this study are discussed based on the distribution of the Oil sands operations for 2035 in the presence of uncertainty in fuel costs and SOR parameters, respectively. The key findings of this study are that oil producers that include hydrocracking are favored over thermocracking-based schemes; *in-situ* (SAGD) operations will play a significant role in the production scenario of the Oil Sands and the GHG emission constraint cannot be met for SOR values higher than 2.48 for the year 2035. These results show that the new extended energy model is a practical tool for determining the energy production costs of the industry, evaluating future environmental policies and energy scenarios, and identifying the key parameters that affect the Canadian Oil Sands operations.

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Detecting bifurcation behaviour in car crash simulation data sets with a generative machine learning method

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Nowadays, the computer simulation of car crashes is an indispensable step in the process of safety analysis and the overall product development for new car models. The assessment of the simulation results by an engineer is still done manually by inspecting one simulation run at a time. Therefore, there is a substantial need to aid the engineer by machine learning methods to significantly reduce the model complexity and detect bifurcations in the course of the simulations. A first approach considering linear dimensionality reduction with a principal component analysis (PCA) for crash simulation data was introduced in [1]. Recent results showing the need for nonlinear methods in this context are given in [2].

In this talk, we will shortly introduce a nonlinear generative method based on [3, 4] and present the workflow for our simulation analysis. The advantage of a generative dimensionality reduction method over other learning algorithms is the ability to inherently map new low-dimensional latent space points into the high-dimensional ambient space. We will show how to use this feature to measure the quality of a constructed embedding of a crash simulation data set. Furthermore, we will present first results on the bifurcation detection with our method and compare the approach to the PCA.

This talk is partly based on collaborative work with Ulf Schepsmeier & Benjamin Peherstorfer (TU Munich), Victor-Rodrigo Iza-Teran, Jochen Garcke & Clemens-August Thole (Fraunhofer SCAI) and Michael Griebel (U Bonn). The corresponding project *SIMDATA-NL* is funded by the German Federal Ministry of Education and Research.

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Effect of Anisotropy on the Steady State Creep in a Rotating Cylinder

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The effect of anisotropy on the steady state creep behavior of a thick-walled rotating circular cylinder made of Al-SiC_p composite subjected to internal and external pressure is investigated in the present study. The creep behavior of the cylinder is assumed to follow Sherby's model [1]. The stresses and strain rates are estimated for the cylinder using Hill's yield criterion [2] for different values of anisotropic parameter (α), characterized by the ratio of radial (or axial) and tangential yield strength of the composite and are also estimated for a similar cylinder but made of isotropic composite. The study revealed that the tangential as well as radial strain rates are significantly affected by the anisotropy of the material. The tangential strain rates are decreased almost by three orders of magnitude in cylinder with anisotropy parameter $\alpha < 1$ as compared to the strain rates obtained for the cylinder with anisotropy parameter $\alpha > 1$. Therefore, it is suggested to use the material having the anisotropy parameter $\alpha < 1$ while designing the cylinder.

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Supply Chain Flexibility Metrics Evaluation

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The markets in which manufacturers and service firms compete are increasingly influenced by intense foreign competition, rapid technological change and shorter product life-cycles. In this new scenario, flexibility may be one of the most important capabilities needed for firms to achieve competitive advantage [1, 2, 3]. We defined flexibility as the capacity of adaptation under the double constraints of uncertainty and the urgency. This uncertainty can come from the providers (rupture, problems of transport), from the customers (variation of the request) or from the company itself (breakdowns of the equipment, problems of provisioning). The possible behaviors of the company face to these problems are called levers of flexibilities. In a supply chain the flexibility of one entity is highly dependent on the flexibility of upstream entities. The overall flexibility of a supply chain will therefore depend on the flexibility of all the entities in a supply chain, and their interrelations. Supply Chain Management (SCM) requires management of complex dependencies between teams, departments and partner companies across international boundaries. It is a natural area for metrics. A metric is a standard of measurement of performance and gives the basis on which to evaluate the performance of processes in the supply chain [4]. Thus the purpose of the study is to determine and evaluate the supply chain flexibility metrics in order to calculate the benefit of preferring a flexibility lever to another one. Then, with respect to increasing benefits, an appropriate flexibility portfolio has to be determined.

We are handling the automotive sector for the study. Automobile manufacturers today compete in an increasingly global environment. A vehicle could be designed in one location and built somewhere else. Components could come from another location, and final assembly could take place in yet another. Fortunately, it's getting easier to work on a worldwide basis, in part because of regulatory and legislative convergence around the globe. The next step includes the convergence of technologies, business practices and lifecycles, and a level of flexibility that enables manufacturers to react quickly.

Measuring flexibility is obviously hard. Thus, to determine the right metrics to use is the first challenge. This step has to be realized with a strong literature survey and operational experts view support. The second step is concerned with the evaluation of chosen metrics. One of the commonly observed methods is fuzzy arithmetic due to the vagueness of some data. The final step is to decide which flexibility levers to use according to the increasing benefits.

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Interdisciplinary Conference Series:
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An Input-Output Analysis Approach in Waste of Electrical and Electronic Equipments

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The production of electrical and electronic equipments is one of the fastest growing markets all over world. Hence, the increasing amount of Waste of Electrical and Electronic Equipments (WEEE) has become a common problem. WEEE has been identified as a priority area to take specific measures on a European scale, particularly the European Commission is among the most active regulators seeking to address the environmental impact of EEE. EU, with the WEEE directive [1] and subsequently amended by [2] and [3], is taking serious measures to prevent the generation of electrical and electronic wastes and to promote reuse, recycling and other forms of recovery in order to reduce the quantity of wastes.

In this study, we focus on waste management and we concentrate on the recycling of mobile phones. Besides the technological developments and the spread of electronic and electrical equipments in many different areas, the mobile phones have dramatically penetrated into the human life and the mobile phone market which has witnessed explosive growth since their introduction is also one of the fastest growing consumer markets. Mobile phones' components and their requirements in production phases such as energy, labor and know-how are depicted in a matrix form inspired from the seminal work of Leontief and an Input-Output (IO) methodology which appears to be appropriate for analyzing waste management problem is presented. IO models have some major extensions in literature as a Physical IO table, Monetary IO table, Waste IO Table and Environmental IO Table. The first one provides a framework in which all physical flows associated with an economy can be recorded, while the second gives an insight into the value of economic transactions between different sectors. Moreover, the third represents the interdependence between the flow of goods and the flow of wastes and the last emphasizes a suitable tool for estimating the short-term response of emissions and resource usage to changes in consumption and production induced by economic growth or by changes in environmental policy [4].

Thus, we propose numerically both static and dynamic input-output solutions in order to put forward the contribution of recycling of mobile phones into the economy. Particularly, we concentrate on the Monetary IO Table with recycling and balance equations. By defining waste outputs as a new vector class, the classical input-output model has been improved. We propose a case study based on approximate data involving the monetary input-output matrix of a manufacturing process of mobile phones and hence, we represent the numerical results of the model. We conclude our paper with the interpretations of graphics, obtained by the model, that numerically emphasize the importance of recycling of the mobile phones.

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Strip-saturation-yield model for a piezoelectric plate - A study on influence of change in poling direction

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It is well-known that a wide range of poled piezoelectric ceramics retains their aligned electric dipole field in the material microstructure below Curie temperature. This electric poling direction effects the material properties and fracture behavior.

It is observed that the presence of crack or cracks considerably reduces the strength of the ceramics. And effect of both mechanical and electric loads is noticeable on crack opening/closing. A vast variety of crack problems for piezoelectric ceramics have been investigated considering impermeable, permeable electric conditions on the crack faces. It is noted that these conditions give higher and lower estimate of energy release rate etc. But empirically it is observed that semi-permeable crack face boundary condition give more accurate results. These may be defined inside crack gap with non-zero permittivity air/dielectric media as

$$D_2^+ = D_2^-, \qquad D_2^+(u_2^+ - u_2^-) = \varepsilon_a(\phi^- - \phi^+), \tag{1}$$

where D_2, u_2, ϕ and ε_a, respectively, denote the electric-displacement, mechanical-displacement components perpendicular to the crack, electric potential and permittivity of media inside crack gap. The superscripts $+$ and $-$ denote the value of quantity over upper and lower faces of the cracks.

The question of arbitrary/changing poling direction on a cracked piezoelectric media under semi-permeable boundary condition on crack is addressed. In the present work, a poled piezoelectric medium is cut along two equal collinear straight cracks. The cracks are assumed to be traction free and inside cracks gaps the semi-permeable boundary condition (1) are assumed to be held. Combine in-plane uniform constant normal (to the faces of cracks) mechanical and electrical-displacement are prescribed at remote boundary of the plate. Consequently cracks open in self-similar fashion forming a yield zone and a saturation zone ahead each tip of the cracks. Its assumed saturation zone and yield zone developed at each tip of the cracks are of equal length. To stop the crack from further opening the developed zones are subjected to in-plane, normal, cohesive saturation limit electric-displacement $D_2 = D_s$ and yield-point stress $\sigma_{22} = \sigma_s$. The mathematical model is obtained using Stroh formalism and solved using complex variable technique. Closed form expressions are derived for crack opening displacement (COD), crack opening potential drop (COP), energy release rate (ERR), lengths of developed zones.

A case study is presented for poled PZT-5H ceramic using proposed model. The effect of change in poling direction is plotted for COD, COP and ERR. It is observed that when poling direction is perpendicular to the crack faces COD, COP and ERR are maximum. And when poling direction is moved along the length of the crack these quantities attain minimum values. A comparative study is presented for impermeable, permeable and semi-permeable cracks cases. It is observed that presence of electric field inside crack gap should not be ignored for design purpose. A study is also presented for COD, COP and ERR to show the mutual effects of two cracks lying close to each other or moved away. The results obtained affirm that poling direction assists in crack arrest under small-scale mechanical yielding and electric saturation.

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Effect of Particle Gradient on the Creep of an Isotropic Rotating Disc

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The effect of imposing linear and non-linear composition gradients on the steady state creep behavior of a rotating functionally graded Al-SiC_p disc is investigated in the present study. Mathematical model to describe steady state creep behavior in rotating discs made of isotropic aluminum composite containing linear and non-linear distributions of Silicon Carbide in the radial direction has been formulated. The steady state creep behavior of the discs has been determined following Sherby's model [1] using von Mises yield criterion [2]. The distributions of stresses and strain rates have been obtained and compared for various functionally graded material (FGM) discs containing the same average amount of dispersoid. The creep response of a composite disc with uniform SiC_p content has also been computed for comparison with the results obtained for FGM discs. The study reveals that the distribution of stresses and strain rates in a rotating composite disc are significantly affected by different particle distributions within the disc. The stresses and steady state strain rates in a rotating FGM disc can be significantly reduced by optimal distribution of SiC_p particles in the disc.

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Hybrid Energy Harvesting Using Piezoelectric and Magnetostrictive Material

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Vibrations energy harvesters have been investigated by many researchers in recent years; typically, energy harvesting systems utilize electromagnetic, piezoelectric, and magnetostrictive technologies. Proposed in this paper is a hybrid energy harvesting unit that employs both piezoelectric and magnetostrictive technologies.

Both piezoelectric and magnetostrictive layers employ a spiral geometry. The spiral shape was previously used by Hu and Xue [1] for a piezoelectric harvester to reduce the natural frequency of the unit. When magnetostrictive material is strained, it introduces a change in the magnetic field of the material. If a copper wire coil is used, through Faraday's law of induction, voltage will be induced in the coil. Some work has been done with this kind of material by Wang and Yuan [2]. The advantage of the proposed design is that it employs both technologies in one unit which results in more efficient harvesting for a wider range of frequencies. Additionally, the spiral shape geometry of the layers helps with the reduction of the natural frequency and allows more efficient harvesting at low frequencies.

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Computational Analysis of Slender Body with Varying Elliptical Cross Section at Various AOAs

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Slender body theory in fluid flow has been developed over last many years ,however discrepencies in aerodynamic forces are noted on fat bodies with elliptical cross section[1]. This research focuses on the CFD analysis of slender body with tri axial elliptical frontal shape. Steady, uniform and incompressible flow with standard sea level conditions is assumed which is alligned with body lateral axis. The analysis has been carried out on bodies of cross section having ellipticity ratios of 0.125,0.25,0.375,0.5,0.75 with wide range of AOAs. Ellipiticity here is defined as the ratio of major axis to minor axis of ellipse (a/0.16) as shown in figure 1. The length of selnder body and major axis of ellipse are kept constant at 0.8m and 0.16m respectively to ensure its slenderness(a/L< 1). Aerodynamic forces on a body with 0.375 ellipticity are compared with experimental work[2] and found in good agreement. Geometry of the body is modelled and meshed in ICEM CFD whereas simulation are run in commercially available software (Fluent). Aerodynamic forces thus obtained from CFD analysis are compared with Oseen flow slender body theory [3]. It is observed that change of turbulence model does not change the basic flow pattern around the slender body however SA turbulence model gives better results when compared with experimental values in lesser number of iterations. It is found that coefficient of lift(C_L) and Lift to drag ratio(L/D) varies directly with angle of attack(α). However the slope of these two curves(C_L Vs α and L/D Vs α) decrease with increase in ellipticity. Body with higher ellipticity ratio produces stronger counter rotating vortices which are captured and presented in this study.

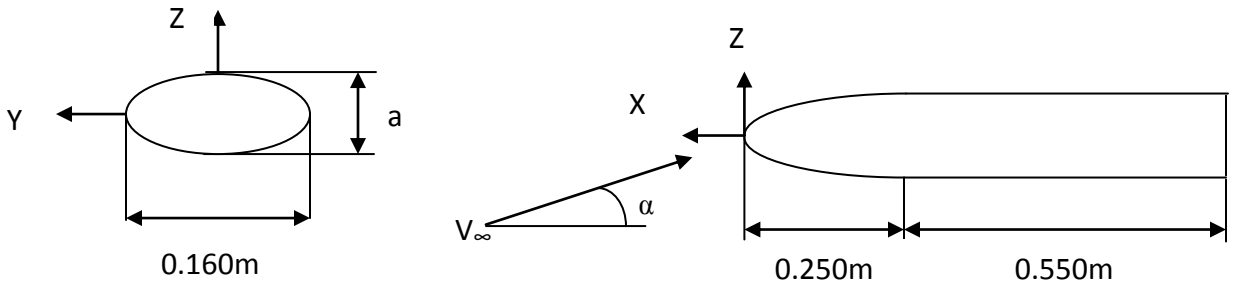

Figure 1: Basic Shape of Slender Body.

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Partial Differential and Integral Equations in Mathematical Modeling (CS-MODELING)

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On Optimal Vortex Structures for Palinstrophy Generation

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We investigate the sharpness of analytic estimates for the growth of palinstrophy $\mathscr{P}$ in the context of the incompressible 2D Navier–Stokes equation defined on $\mathbb{T}^2$. This problem is a 2D counterpart of the problem concerning the maximum growth of enstrophy $\mathscr{E}$ in 3D Navier–Stokes flows, which is inherently related to the question of finite–time singularity formation [1].

Using standard methods of analysis, it is possible to find estimates for the rate of growth of palinstrophy $d\mathscr{P}/dt$ and the maximum palinstrophy $\mathscr{P}_{\max} := \max_{t>0} \mathscr{P}(\omega(\cdot,t))$ in the form:

$$\frac{d\mathscr{P}}{dt} \leq C_0 \mathscr{K}^{1/2} \mathscr{P}^{3/2}, \tag{1}$$

$$\mathscr{P}_{\max} \leq C_1 \mathscr{K}_0 \mathscr{E}_0^2, \tag{2}$$

where ω is the scalar vorticity, C_0 and C_1 are positive constants, $\mathscr{K}(\cdot)$ denotes energy and $\mathscr{K}_0$ and $\mathscr{E}_0$ in (2) correspond to the energy and enstrophy at time $t = 0$, respectively. Optimal vorticity fields $\tilde{\omega}$ are found by solving numerically optimization problems of the form:

$$\tilde{\omega}_{\mathscr{K}_0,\mathscr{P}_0} = \operatorname*{arg\,max}_{\omega \in \mathscr{Q}_{\mathscr{K}_0,\mathscr{P}_0}} \frac{d\mathscr{P}}{dt}, \tag{3}$$

$$\mathscr{Q}_{\mathscr{K}_0,\mathscr{P}_0} = \left\{ \omega \in H^2(\mathbb{T}^2) : \mathscr{K}(\omega) = \mathscr{K}_0, \mathscr{P}(\omega) = \mathscr{P}_0 \right\},$$

where the parameters $\mathscr{K}_0$ and $\mathscr{P}_0$ range over several orders of magnitude, and we provide evidence supporting the sharpness of the instantaneous estimate in (1).

Additionally, numerical simulations of the 2D Navier–Stokes flow with $\tilde{\omega}$ as initial data, indicate that $\mathscr{P}_{\max}$ features the same power–law behaviour with respect to $\mathscr{E}_0$ as predicted by the finite–time estimate (2), suggesting that the vortex structures that saturate the instantaneous estimate are also optimal for the finite–time estimates [2].

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Global Existence and Blow-up of Solutions for a Class of Nonlinear Nonlocal Wave Equations

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We mainly deal with local existence, global existence and blow-up results for solutions of the Cauchy problem

$$u_{tt} - Lu_{xx} = B(g(u))_{xx}, \quad x \in R, \quad t > 0, \tag{1}$$
$$u(x,0) = \varphi(x), \quad u_t(x,0) = \psi(x), \tag{2}$$

where g is a sufficiently smooth nonlinear function, L and B are linear pseudodifferential operators defined by

$$\mathscr{F}(Lv)(\xi) = l(\xi)\mathscr{F}(v)(\xi), \quad \mathscr{F}(Bv)(\xi) = b(\xi)\mathscr{F}(v)(\xi).$$

Here $\mathscr{F}$ denotes the Fourier transform with respect to variable x and $l(\xi)$ and $b(\xi)$ are the symbols of L and B, respectively. We assume that L is an elliptic coercive operator of order ρ with $\rho \geq 0$ while B is an elliptic positive operator of order $-r$ with $r \geq 0$. In terms of $l(\xi)$ and $b(\xi)$, this means that there are positive constants c_1, c_2 and c_3 so that for all $\xi \in R$,

$$c_1^2(1+\xi^2)^{\rho/2} \leq l(\xi) \leq c_2^2(1+\xi^2)^{\rho/2},$$
$$0 < b(\xi) \leq c_3^2(1+\xi^2)^{-r/2}.$$

Local existence of solutions of the Cauchy problem (1)-(2) with initial data in suitable Sobolev spaces is proven and the conditions for global existence and finite-time blow-up of solutions are established.

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Symbolic - Numerical Methods For Some Special Functions Involved in Groundwater Hydrodynamics

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Groundwater makes up almost 30better understanding of the system are difficult to validate due to the disordered nature of the porous media and the complex geometry of the channels of flow, Refs. [4].

In this talk I will first establish the general 3D groundwater equations as expressed in Eqs. (1)

$$\frac{\partial}{\partial x}(K_x\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}(K_y\frac{\partial h}{\partial y})+(K_x\frac{\partial h}{\partial z})=S_s\frac{\partial h}{\partial t} \tag{1}$$

Where:
$h=$ the hydraulic head
$K=$ the hydraulic conductivity
$S_s=\rho g(\alpha+nB)$, the specific storage, with:
$\alpha=$ the compressibility of aquifer
$B=$ the compressibility of water
$\rho g=$ the specific weight of the water
$n=$ the porosity

By transforming the Eqs. (1) in different coordinate systems, I will show that dependant of the initial and boundary conditions, the solutions of Eqs. (1) could be expressed in term of special functions like Bessel, Error, Polder, Airy, Henkel and others related special functions in term of their asymptotic expansions Refs. [1,2,3,5]. These functions above are of considerable importance for solutions of radial-symmetric and axial-symmetric flow. I will also describe and verify by an experimental technique an algorithm for computing the Bessel functions $J_\mu^{(\mu T)}, Y_\mu^{(\mu T)}$ and their derivatives by using the modern Computer Algebra System Refs. [3] in the neighborhood of the turning point for large values of the parameters. The results obtained could help for a better planning, engineering and management of the groundwater hydrology.

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Symmetry classification of a generalized variable-coefficient Gardner equation

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We make an analysis of the symmetry reductions of a generalized variable-coefficient Gardner equation by using the classical Lie method of infinitesimals. The direct method of group classification is utilized to specify the forms of these time-dependent coefficients.

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Numerical simulation of potential Maxwell's equations in harmonic regime[1]

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In this work we are concerned with the following nonlinear PDEs system

$$\left.\begin{aligned}
&-\nabla\cdot(\sigma(\theta)\nabla\varphi) = i\lambda\omega\nabla\cdot(\sigma(\theta)\boldsymbol{A}) + f \text{ in } \Omega_T = \Omega\times(0,T),\\
&i\omega\sigma(\theta)\boldsymbol{A} + \nabla\times\left(\tfrac{1}{\mu}\nabla\times\boldsymbol{A}\right) - \delta\nabla(\nabla\cdot\boldsymbol{A}) = -\sigma(\theta)\nabla\varphi \text{ in } D_T = D\times(0,T),\\
&\varphi = 0 \text{ on } \Gamma_0\times(0,T), \quad \frac{\partial\varphi}{\partial n} = 0 \text{ on } \Gamma_1\times(0,T), \quad \boldsymbol{A} = 0 \text{ on } \partial D,\\
&\theta_{,t} - \nabla\cdot(\kappa(\theta)\nabla\theta) = \frac{\sigma(\theta)}{2}|i\omega\boldsymbol{A} + \nabla\varphi|^2 + G \text{ in } \Omega_T,\\
&\frac{\partial\theta}{\partial n} = 0 \text{ on } \partial\Omega\times(0,T), \quad \theta(\cdot,0) = \theta_0 \text{ in } \Omega.
\end{aligned}\right\} \tag{1}$$

This system describes the heating stage of the induction–conduction industrial procedure applied to a steel workpiece ([2]-[5]). In this framework, $\Omega, D \subset \mathbb{R}^3$ are bounded, connected and Lipschitz–continuous open sets such that $\bar{\Omega} \subset D$, $\partial\Omega = \Gamma_0 \cup \Gamma_1$ and $\partial D = S_0 \cup S_1$, the unknowns are the electric potential, φ, the magnetic vector potential, $\boldsymbol{A}$, and the temperature, θ; σ and κ are the electric and thermal conductivities, respectively, ω is the angular frequency (about $1.6\pi 10^6$), θ_0 the initial temperature, i stands for the imaginary unit, and μ is the magnetic permeability. Finally, $\lambda \in [0,1]$ and $\delta > 0$ is a small parameter. Problem (1) is referred to as the harmonic regime ([1, 4, 5]). In this way, both φ and $\boldsymbol{A}$ are complex-valued scalar and vector fields, respectively.

The original value for the parameter λ is $\lambda = 1$, but in most numerical simulations the value $\lambda = 0$ is taken which yields to an enormous reduction of computational cost. In [5], the authors have shown the existence of a weak solution to (1) in the range $0 \le \lambda < 1 - \frac{1}{\omega}$, so that $\lambda = 1$ is not attainable!

We have carry out some numerical experiments for the resolution of the linear system φ-$\boldsymbol{A}$ for a given temperature. We have used a Crank-Nicolson like iterative scheme which compute, for a given $\boldsymbol{A}^0$, φ^0, then $\boldsymbol{A}^1$ and φ^1 and so on. The numerical results show a strong relation between λ and the rate of convergence of this scheme: the closer the value of λ to 1, the more number of iterations are needed.

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Kinetic and Material Property Effects on Fingering Instability in Reverse Smoldering Combustion

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Based on one-temperature equilibrium combustion models (see Eqs. (1)-(3), and Ref. [1]) derived through the mathematical theory of periodic homogenization, we study numerically the consequence of kinetic and material property on the developed fingering state. In a previous study [1], we showed that material thermal effects are not the controlling mechanism underlying the combustion instability. In this presentation, we focus on the effects of system porosity ϕ and heat release on the developed fingering state i.e. we consider the tip-splitting regime of the instability (see Refs. [1, 2] for details). In the first case, we show qualitative numerical results that relates ϕ to the depth of conversion of the solid product. In order to investigate the implication of heat release on the characteristic finger width via an adiabatic model that neglects heat release mechanisms e.g. radiative heat transfer, the rate of heat released at the reaction zone is controlled. We show the dependence of the finger width on the ability of the front to release heat (see Fig. 1) , thereby justifying qualitatively the experimental observation relating the finger width to heat released by the front [2].

$$\frac{\partial T}{\partial t} - \nabla^2 T + \phi \Lambda Pe \cdot \nabla T = ANCe^{N(1-1/T)}, \tag{1}$$

$$\phi \frac{\partial C}{\partial t} - \frac{1}{Le}\nabla^2 C + \phi Pe \cdot \nabla C = -ANCe^{N(1-1/T)}, \tag{2}$$

$$\frac{\partial R}{\partial t} = H_R ANCe^{N(1-1/T)}. \tag{3}$$

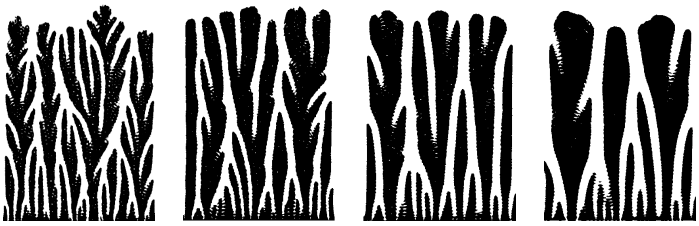

Figure 1: Collage of fingering char patterns in the tip-splitting regime showing variation of finger width with decreasing values of A (i.e. from left to right) and fixed values of Pe and Le. Ignition is initiated from bottom; char propagation is from bottom to top.

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Coupled Heat Transport and Darcian Water Flow in Freezing Soils

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This contribution deals with a model of coupled heat transport and Darcian water flow in unsaturated porous media taking into account the effects of freezing and thawing. Let Ω be a bounded domain in $\mathbb{R}^N$, $N = 1,2,3$, occupied by a partially saturated soil and I be any physically relevant time interval. The model consists of the following balance equations (see [1, 2, 3]):

the conservation equation for total mass of liquid water and ice:

$$\frac{\partial(\rho_\ell \theta_\ell)}{\partial t} + \frac{\partial(\rho_i \theta_i)}{\partial t} = -\nabla \cdot (\rho_\ell \theta_\ell \mathbf{v}_\ell) \quad \text{in } \Omega \times I; \tag{1}$$

and *energy conservation equation:*

$$c_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) - c_p^\ell \rho_\ell \theta_\ell \mathbf{v}_\ell \cdot \nabla T - L_f \frac{\partial(\rho_i \theta_i)}{\partial t} \quad \text{in } \Omega \times I, \tag{2}$$

which are supplemented with appropriate boundary and initial conditions for calculating water and heat fluxes across the boundary of Ω and initial distributions of temperature and water content in Ω. The unknowns in the model are the total pressure head $u = u(\mathbf{x},t)$ [m] and temperature $T = T(\mathbf{x},t)$ [K] (single-valued functions of the time t and the spatial position $\mathbf{x} = [x,y,z] \in \Omega$). Further, $\theta_\ell = \theta_\ell(z,u,T)$ [-] represents the volumetric unfrozen water content, $\theta_i = \theta_i(z,u,T)$ [-] is the volumetric ice content, $\mathbf{v}_\ell$ [$\mathrm{m\,s^{-1}}$] the velocity of the flow of unfrozen water, $c_p = c_p(z,u,T)$ [$\mathrm{J\,m^{-3}\,K^{-1}}$] is the volumetric heat capacity of the soil and $\lambda = \lambda(z,u,T)$ [$\mathrm{W\,m^{-1}\,K^{-1}}$] represents the effective thermal conductivity of the soil. Material constant parameters are the volumetric heat capacity of water c_p^ℓ [$\mathrm{J\,m^{-3}\,K^{-1}}$], the density of liquid water ρ_ℓ [$\mathrm{kg\,m^{-3}}$], the density of ice ρ_i [$\mathrm{kg\,m^{-3}}$] and L_f represents the latent heat of fusion [$\mathrm{J\,kg^{-1}}$].

We employ the Rothe method to construct approximate solutions to the model and prove some results concerning the existence and regularity of the numerical solution. Finally, we also present some illustrative numerical examples.

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High Concentration Vesicle Suspensions

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We define a vesicle $\gamma \in \mathbb{R}^2$ to be a closed, inextensible, lipid membrane. Vesicles are used to model different bio-physical elements such as red blood cells. We consider vesicles that are submerged in a domain Ω of incompressible, viscous fluid. The equations that govern the fluid and the vesicle dynamics are [1]

$$\begin{aligned} \Delta \mathbf{u} - \nabla p &= 0, & \mathbf{x} &\in \Omega \backslash \gamma, \\ \nabla \cdot \mathbf{u} &= 0, & \mathbf{x} &\in \Omega \backslash \gamma, \\ \mathbf{u} &= \mathbf{f}, & \mathbf{x} &\in \partial\Omega, \end{aligned} \qquad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{u}, & \mathbf{x} &\in \gamma, \\ div_\gamma \dot{\mathbf{x}} &= 0, & \mathbf{x} &\in \gamma, \\ [\![-pI + \nabla \mathbf{u} + \nabla \mathbf{u}^T]\!] &= \xi, & \mathbf{x} &\in \gamma. \end{aligned}$$

The inextensibility condition, $div_\gamma \dot{\mathbf{x}} = 0$, is satisfied by introducing the tension σ which acts as a Lagrange multiplier. The jump in the stress is $\xi = -\mathbf{x}_{ssss} + (\sigma \mathbf{x}_s)_s$ which minimizes the bending energy of the vesicle.

Integral equation methods have become increasingly popular for solving coupled fluid-solid equations such as the above. The governing equations become a system of integro-differential equations for the position of the vesicle $\mathbf{x}$, the tension σ, and an unknown density function defined on $\partial\Omega$. The advantage of this formulation is that all the unknowns live on one-dimensional curves. However, when vesicles approach one another or a solid wall, several issues must be addressed. The integral operators become difficult to evaluate accurately, the problem becomes stiff, and the number of required GMRES steps increases. To handle high concentrations of vesicles, we use near-singular integration, fast multipole methods, implicit time stepping, and block-diagonal preconditioning.

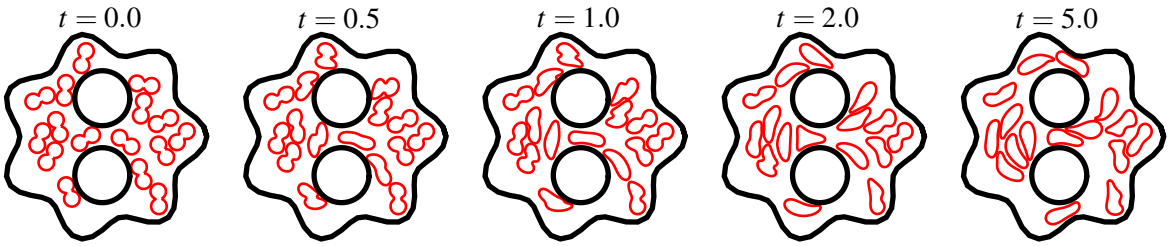

Figure 1: The vesicles (red) and solid walls (black) are each discretized with 64 points. The result is a linear system with 3,456 unknowns that must be solved at each time step. Even with this complex geometry, we are able to achieve an error of 0.05%. The inner boundaries are rotating in opposite directions with constant angular velocity while the outer boundary is fixed. We see that the vesicles are able to come quite close to one another and the solid walls.

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Modelling, Simulation and Optimization of Gas Flow in an Exhaust Pipe

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The emission caused by vehicles is an import issue in these times. In order to reduce the pollutant emissions of CO, NO_x and C_xH_y in the exhaust gas, there are catalytic converters installed in the exhaust pipe system. A crucial quantity to control the efficiency of a catalytic converter is the temperature. Due to this reason, one is interested in how to ensure a sufficient high temperature in the catalytic converter in a short time after the engine start.
We start with the following fully compressible, hyperbolic balance law, which is commen in engineering literature

$$\begin{aligned}
(A\rho)_t + (A\rho u)_x &= 0,\\
(A\rho u)_t + (A\rho u^2)_x + Ap_x &= -\frac{\xi\pi d}{4}\rho\frac{u|u|}{2} - C_c A\chi\rho u,\\
(A\rho E)_t + (A\rho uE + Aup)_x &= -h\pi d(T - T_{\text{Wall}}) + q_0 A\chi\rho z K(T),\\
(A\rho z)_t + (A\rho uz)_x &= -A\chi\rho z K(T),
\end{aligned}$$

where we use the ideal gas law $p = R\rho T$ as the closing relation. The terms on the left hand side are the Euler equations of gas dynamic in a pipe with a variable cross section A. By the terms on the right hand side we describe the main physical effects which influence the dynamic of the gas.

Starting from this model we perform two major simplification in our work:

1. Rather than introducing intervals for a smooth change of the cross section A, we divide the exhaust pipe into pipes with constant cross sections and treat the whole system as a network. This has two major advantages:
   (a) Since the cross section A does not have to change quickly on small intervals, which would imply large derivatives, we are able to produce numerical results with much larger step sizes in space.
   (b) Due to the necessity of coupling conditions for the network, we are able to describe the pressure losses caused by the pipe's geometry.
2. The flow in the exhaust pipe is in a low Mach number regime, and we are not interested in the propagation of sound waves, but mainly the temperature in the catalyst. Thus, we are able to simplify the model by a small Mach number asymptotics. This will lead us to a simplified model, which is computationally much faster than the hyperbolic model, since much larger step sizes in time are allowed by the CFL condition.

Furthermore we will present a related optimisation problem: Heating up the catalytic converter as fast as possible without using too much fuel.

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Convergence of the Lagrange-Galerkin method for the equations modelling of fish-like swimming

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We focus on a numerical method for the disctretization of an initial and boundary value problem that models the self–propelled motion of a deformable solid in a bidimensional viscous incompressible fluid. In the model, we suppose that the solid is subjected to a known deformation field representing the action of the aquatic organism muscles. The governing equations consist of the Navier–Stokes equations for the fluid, coupled to Newton's laws for the solid. The numerical method we propose is based on a global weak formulation, where the nonlinear term in the Navier–Stokes model is discretized using the characteristic function. Since the formulation is global in space, this characteristic function is extended in an appropriated manner inside of the creature, taking into account its deformation. We first concentrate our attention in the semi–discretization in time and we prove the stability and the convergence of the scheme. The numerical method is consistent enough with the motion of the creature and for this reason, the disctretization in space variable is successfully implemented using finite element method.

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Bounds on dispersion tensor in periodic media

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In this talk, we consider a periodic media and we study the dependence of the dispersion tensor or Burnett coefficients in terms of the microstructure (for the definition of this tensor, we refer the reader to [1] and [2]). We treat one-dimensional and laminated structures, and also we give some perspectives on other cases in higher dimension. In low contrast periodic media, interesting properties of the sign of this tensor are found. Surprisingly, these depend on the microstructure only through the local proportion parameter and in some cases, they do not depend on the microstructure at all. Considering the general one dimensional periodic medium, we completely describe the set in which the dispersion coefficient lies, as the microstructure varies preserving the volume proportion (see [3]). In higher dimension, we study properties on the dispersion tensor for laminated (see [4]) and Hashin structures and we characterize the bounds of this tensor in terms of some geometric properties on the reference cell.

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Mixed problems for the Telegraph Equation in the Case of a System Consisting of N Segments with different Densities and Elasticities but Equal Impedances

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We consider the mixed problems for the longitudinal vibrations of a rod governed by the telegraph equation with the Dirichlet and Neumann boundary conditions. The rod consists of n segments with different densities and elasticities.

The rod has the linear density $\rho_1 = const$ and Young's modulus $k_1 = const$ on the segment $0 \le x \le l_1$.

The rod has the linear density $\rho_i = const$ and Young's modulus $k_i = const$ on the segment $l_{i-1} \le x \le l_i$.

The rod has the linear density $\rho_n = const$ and Young's modulus $k_n = const$ on the segment $l_{n-1} \le x \le l_n = l$.

The impedances of these n segments are equal to each other.

The study of the vibrations of the rod subject to the given boundary conditions at its ends is reduced to finding the solution u(x, t) of the following mixed problem for the discontinuous telegraph equation with $a_i = \sqrt{\frac{k_i}{\rho_i}}$

$$u_{tt} = \{ a_i^2 u_{xx}(x,t) + c^2 u(x,t) \text{in } Q_2 = [l_{i-1} \le x \le l_i] \times [0 \le t \le T], \tag{1}$$

with zero initial conditions

$$u(x,0) = 0, \quad u_t(x,0) = 0, \tag{2}$$

with junction conditions at the joint points $l_i, i = 1 \ldots n$,

$$u(l_i - 0, t) = u(l_i + 0, t), \quad k_i u_x(l_i - 0, t) = k_{i+1} u_x(l_i + 0, t) \tag{3}$$

and with one of the following three pairs of boundary conditions:

$$u(0,t) = \mu(t), \quad u(l,t) = \nu(t), \tag{4^1}$$

(displacements at both ends);

$$u_x(0,t) = \mu(t), \quad u_x(l,t) = \nu(t), \tag{4^2}$$

(elastic forces at both ends), and

$$u_x(0,t) = \mu(t), \quad u(l,t) = \nu(t), \tag{4^3}$$

(an elastic force at one end and a displacement at the other).

Further, the paper presents a practical application of the explicit formulas for the solution of the above mixed problems for solving and modeling seismic migration problems in a dispersion medium.

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On a Two-Fluid Slot Coating Flow with Evaporation

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In this paper a particular plane steady-state slot coating flow including evaporation effects is investigated. The motion of two heavy viscous immiscible fluids is governed by a free boundary value problem for a coupled system of Navier-Stokes and Stephan equations. The flow domain is unbounded in two directions and both of the free interface/surface are semi-infinite. It contains two sharp corners where the weak solution admits singularities. Existence and uniqueness of a suitable solution in weighted Hölder spaces can be proved for small data (i.e. small fluxes) of the problem.

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A Mathematical Cellular Pott's Model for Growth and Migration of Endothelial Cells

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Several studies have suggested mathematical models that simulate growth and migration of endothelial cells and capillary network formation in angiogenesis[1-2]. The target is to predict endothelial cells and constructed capillary network behavior in different cellular environmental conditions. This study presents a cellular Pott's model to simulate an endothelial cell growth and migration. The extracellular matrix affects the cell through environmental signals which are chemical and mechanical. Chemical signals activate cell receptors and start changes in cells' internal machinery. It is considered that the main signaling agent in the extracellular matrix is tumor angiogenic factor (TAF) that is released by tumor. Mechanical signals are created due to interaction of cell receptors and extracellular matrix elements like fibers. The matrix elements are also the main coordinators of endothelial cell movement.

Using the Pott's model for cellular dynamics, growth and migration of an endothelial cell integrated with the signals cell receive from the environment. The results of the model predict cell migration and growth based on environmental cues. Chemotactic movement of the endothelial cell in response to the TAF gradient is seen clearly in this model. The results of this model can be extended to multiple endothelial cells and in next steps, to simulate a capillary and eventually, network formation.

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A free boundary approach to solve the equilibrium equations of a membrane

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This work presents a mathematical problem related to the equilibrium analysis of a prestressed membrane with rigid and cable boundaries. The membrane is represented by a regular surface $z(x,y)$, defined in a bounded domain $D \subset \mathbb{R}^2$, and its boundary by a set of regular curves; Γ^{r} and Γ^{c} represent the rigid and the cable boundary, respectively ($\partial D = \Gamma^{\mathrm{c}} \cup \Gamma^{\mathrm{c}}$). Equilibrium is directly expressed by means of a second order boundary problem in terms of the membrane and its positive (tension) stress tensor $\sigma(x,y)$. The membrane-cable interface equilibrium requires taking into account a singular condition that makes the problem more difficult.

Precisely, if H represents the Hessian matrix of z and t is the tangent unit vector to Γ^{c}, we have to find z such that

$$\begin{cases} \operatorname{div}(\sigma \cdot \nabla z) = 0 \text{ in } D, \\ z = g \text{ on } \Gamma^{\mathrm{r}}, \\ t \cdot (H \cdot t) = 0 \text{ on } \Gamma^{\mathrm{c}}, \end{cases} \tag{1}$$

σ and g being two given functions defined in D and Γ^{r}, respectively. In order to solve this problem, we propose to take into account another unknown function h on Γ^{c} and, also, to consider Γ^{c} as a free boundary of ∂D. If we impose the function h to be equal to z on Γ^{c} a different formulation, but totally equivalent, of (1) is obtained. As a consequence, using a fix point procedure, it is possible to fit the shapes of the cable (i.e. Γ^{c}) and of the membrane (i.e. z) so that system (1) is completely verified.

Finally, some numerical results related to the corresponding free boundary algorithm are presented and discussed.

Acknowledgements

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Poster Session (CS-POST)

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Finite Element Approximation of a Parabolic Cross-Diffusion System

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A mathematical and numerical analysis will be carried out for a nonlinear parabolic cross diffusion system: Find $\{w(x,t),z(x,t)\} \in [-1,1] \times R$ such that

$$\frac{\partial w}{\partial t} = \nabla \cdot \left(\rho \nabla w - (1-w^2) \nabla z \right) \quad \text{in } \Omega_T, \tag{1}$$

$$\frac{\partial z}{\partial t} = \nabla \cdot (\nabla z + \lambda \nabla w) + \mu w - z \quad \text{in } \Omega_T, \tag{2}$$

where $\Omega = (0,L) \subset R$ for some $L > 0$, and $\Omega_T := \Omega \times (0,T)$ for positive time $T > 0$.

The above system models axial separation of a mixture of two sorts of particles, A_1 and A_2, in a long rotating drum with length $L > 0$. Here $w = w_{A_1} - w_{A_2} \in [-1,1]$ is the relative concentration of the mixture, where $w_{A_1}, w_{A_2} \in [0,1]$ are the concentrations of the two particles A_1 and A_2. The variable z represents the so-called dynamic angle of repose which is defined as the angle of the slope of the free surface of grains in the drum as they flow continuously. The constant $\rho > 0$ is related to the Fick diffusion constants arising in the surface fluxes of the two materials, while the positive constant $\lambda > 0$ is proportional to the difference of the Fick diffusivities. Finally, the non-negative constant $\mu \geq 0$ is related to the static angle of repose of the particles.

A regularized fully discrete finite element approximation of the system is proposed and studied. With the aid of a fixed point theorem, existence of the fully discrete solutions is shown. By using entropy-type inequalities and compactness arguments, the convergence of the approximation of the system is proved and hence existence of a global weak solution is obtained. Finally, a practical algorithm for computing the numerical solutions of the system is described and some numerical experiments are performed.

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Convergence of the Regularized Sinc Collocation Method Applied to First kind Fredholm Integral Equation

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In this study one of the new techniques is used to solve numerical problems involving integral equations known as regularized sinc-collocation method. This method has been shown to be a powerful numerical tool for finding accurate solutions. So, in this talk, some properties of the regularized sinc-collocation method required for our subsequent development are given and are utilized to reduce integral equation of the first kind to some algebraic equations. Then by a theorem we show error in the approximation of the solution decays at an exponential rate. Finally, numerical examples are included to demonstrate the validity and applicability of the technique.

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Short-wave vortex instability in stratified flow

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Vortices play an important role in the transition to turbulence, especially in geophysical flow. Of particular interest is the study of stratified turbulence, which occurs when the fluid has non-constant density, such as in the ocean and atmosphere. While stratified turbulence may behave similar to unstratified turbulence initially, its long term behaviour differs due to the stratification [3]. Thus, in addition to the Reynolds number Re, stratified turbulence is also governed by the Froude number $Fr = U/NL$ where U is the characteristic velocity, L is the characteristic length, and N is the Brunt-Vaisala or buoyancy frequency, which is measure of the stratification of the flow. Because of this extra dependence on the Froude number, modelling geophysical flow becomes more complicated as one cannot apply unstratified turbulence models and ideas. Understanding how stratified turbulence differs is important for numerical simulations. A common approach to studying turbulence is to investigate the transition to turbulence in simplified models as it can illustrate key features and behaviour that govern the more complicated turbulent flow.

A popular model used to study stratified flow is that of a columnar counter-rotating dipole. Laboratory and numerical experiments into the stability of such dipoles have uncovered an instability unique to stratified flow, the zigzag instability, so named due to the zigzag-like structure exhibited by the flow[1, 2]. The zigzag instability is a relatively large scale instability appearing with characteristic vertical length of $\sim U/N$. This instability has been verified in other stratified flow models including co-rotating and vortex arrays. However a complete study of the stability of the counter-rotating dipole has not been done and previous research has only focused on large scale vertical length perturbations while the small scale perturbations have been neglected. Our work investigates the stability of these small scales.

In this talk we present and discuss a new instability of the counter-rotating dipole discovered through numerical linear stability analysis. We analyse the growth rate of the Lamb-Chaplygin dipole under the Boussinesq approximations subject to 3D perturbations. The Lamb-Chaplygin dipole is an exact solution to the 2D Euler equations and approximates the laboratory experiments of a counter-rotating dipole. We investigate numerous Reynolds and Froude numbers and a wide variety of vertical perturbations.

This new instability appears at smaller vertical scales than the zigzag instability by about an order of magnitude. However its growth rate is roughly the same, and may even exceed, that of the zigzag instability. Additionally, the structure of the perturbation differs from that of the zigzag instability. This new instability has implications for numerical modelling of small scales in stratified turbulence.

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A Mathematical Model For Treatment Selection

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The changes in the practice of medicine influenced by the evidence based medicine (EBM) model in the last 20 years has promoted greater involvement from patients, other healthcare professionals (e.g., pharmacists, psychotherapists, etc.) and even the community when selecting treatment options or making treatment decisions. During the formulation of a treatment plan, medical factors (such as unstable angina, use of anticoagulants, etc.) certainly have an influence, but they are not the sole influence. Non-medical factors also play an important role in the treatment decision making process for patients, their families and caregivers. Important factors such as the patient's age, living status, level of independence, level of support from medical services such as from a Community Care Access Center (home care) and personal support structures can have a profound influence on the decision making process. Travel and lodging can also be major factors given geographical distribution and disparate population. There may also be a seasonal variation in the availability of treatment as a result of adverse weather conditions. Often factors which are seemingly trivial, (how do you do the dishes if you have an incision on your hand?) are also important. To say nothing of external issues that must be taken into account, such as resource availability and funding scenarios.

In order to reconcile these often disparate and seemingly difficult to quantify factors, a mathematical model utilizing the pairwise comparisons method will be introduced. As will be shown, the proposed model will allow for decisions on the treatment selection to be made with more accuracy and determinism via the weighted analysis of the ratings of the factors by all stakeholders (experts and non-experts alike). The objective of this study will be to demonstration positive impacts on treatment outcome, wait-times, resource usage maximization, physician workload, patient satisfaction and data quality.

By common sense, it is easier to compare factors influencing our treatment decisions two at a time rather than all at once. However, these partial comparisons not only need to be synthesized but also analyzed for inconsistencies. The minimum cycle of such assessments is three (in case of two, it is inaccuracy; not inconsistency). The inconsistency indicator proposed by Koczkodaj in 1993 as $ii = min(|1 - a * c/b|, |1 - b/a/c|)$ for a triad (a,b,c) allows us to localize the most inconsistent triad for reconsideration or reconciliation of assessments. Unlike the eigenvalue-based inconsistency, the distance-based inconsistency localizes the most inaccurate assessments hence allowing for their reconsideration.

The pairwise comparisons method, when leveraged by the collaborative capabilities of the internet and synthesized with the combined input from all stakeholders (individual and organizational), will provide the ideal framework within which a distributed, decentralized model can be created that will provide an accurate, evidence-based assessment of treatment plan selection. The resulting system will provide healthcare professionals, individuals and families with the ability to balance the often disparate factors that contribute to treatment selection, and make informed choices about the proposed treatments.

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A Differential Quadrature Algorithm for Numerical Treatment of Two-Dimensional Hyperbolic Equation

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The hyperbolic partial differential equations model the vibrations of structures (e.g., buildings, beams, and machines) and they are the basis for fundamental equations of atomic physics. The equations are important for modeling several relevant problems such as signal analysis [1], wave propagation [2], random walk theory [3], in many branches of physics, fluid dynamics and aerodynamics, theory of elasticity, optics, electromagnetic etc. In this article, we proposed a numerical technique based on polynomial differential quadrature method (PDQM) to find the numerical solutions of two dimensional hyperbolic equations with Dirichlet and Neumann boundary conditions. The PDQM reduced the problem into a system of second order linear differential equation. Then, the obtained system is changed into a system of ordinary differential equations and lastly, RK4 method is used to solve the obtained system. Numerical results are obtained for various linear and nonlinear hyperbolic equations. The numerical results are found to be in good agreement with the exact solutions and the numerical solutions exist in literature. The technique is easy to apply for multidimensional problems.

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Multiplication Operators with Closed Range in Operator Algebras

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Let $\mathscr{B}(H)$ denote the C^* algebra of all bounded linear operators from a Hilbert space H into itself. Let $T \in \mathscr{B}(H)$. Define $L_T : \mathscr{B}(H) \to \mathscr{B}(H)$ by $L_T(S) = TS$ and define $R_T : \mathscr{B}(H) \to \mathscr{B}(H)$ by $R_T(S) = ST$. Consider the following three statements :

1. T has closed range in H.
2. L_T has closed range in $\mathscr{B}(H)$.
3. R_T has closed range in $\mathscr{B}(H)$.

It is proved that all statements are equivalent. Some possibilities of extending this result to Banach spaces have been discussed.

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Comparing the Results of Transforming Differential Method and Adomian Method in Solving Third Order Nonlinear Delay Differential Equation

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Transforming differential method is a Numerical and Analytical Method for solving functional equations. In this method, Computation is reduced greatly without any linearization, discretezation and making perturbation in problem and leads to an acceptable answer with high accuracy. In this paper, we intend to compare and analysis the transforming differential method and Adomian method in solving third order nonlinear Delay differential equation which is one of the most important Delay differential equation.

Keywords: transforming differential method, functional equations, Adomian method, third order nonlinear delay differential equation.

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Domain interactions from protein interactions with Formal Concept Analysis

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Given a binary relation $I \subseteq G$ x M where G is the set of objects and M is the set of attributes, Formal Concept Analysis (FCA) [1] produces a lattice where each node is a (formal) concept within the (formal) context of I. A concept is an ordered pair (O, A) with extent O and intent A such that $O \subseteq G$, $A \subseteq M$ and the common attributes of O under relation I imply A while the common objects of A under relation I imply O.

The broad objective of my research is to investigate the usefulness of a concept lattice L when G is a set of proteins, M is a set of domains and $(g, m) \in I$ means protein g has domain m, or equivalently domain m occurs in protein g. I believe this is the first application of FCA to proteins and their domains. In this talk, I will present my FCA based approach and results I have obtained so far with respect to the problem of inferring domain-domain interactions (DDI) which underlie a given set of protein-protein interactions (PPI). This is done under the assumption that DDIs explain PPIs (PPIs are explained by other additional factors).

Through concept intents and interaction between concepts, L naturally models intra- and inter- domain combinations. The use of intra- and inter- domain combinations has been shown to improve DDI and PPI predictions [e.g. 4 & 2]. In my approach, a concept pair (c_i, c_j) with $c_i = (O_i, A_i)$ and $c_j = (O_j, A_j)$ produces the pair $(O_i \times O_j, A_i \times A_j)$ where $O_i \times O_j$ is a set of putative PPIs, and $A_i \times A_j$ is a set of putative DDIs. The information from concept pairs and the given set of PPIs are then used to rank concept pairs.

Using the dataset and general methodology published in [3 & 4], and an assumption of 50% reliability for each PPI, the following observations are made:

(i) High ranking concept pairs are enriched with gold standard domain pairs, self-interacting domain pairs and co-occurring domain pairs. This is noteworthy because there is evidence that these types of domain pairs are more likely to interact with one another. The gold standard set of DDIs come from [3]. A domain pair (x, y) is co-occurring if both domains x and y are found in at least one protein in the input set.

(ii) The highest ranking concept pair of a selected PPI is highly likely to contain at least one gold standard domain pair. The selected PPIs come from [3].

These observations indicate that my FCA based approach is applicable to the problem of inferring DDIs that underlie a given set of PPIs. In contrast to [4], my observations were made with Pfam-B domains included. This can be useful to fill in current information gaps about Pfam-B domains. Further, since concept pairs are used instead of individual domain pairs, the role of domain context can be studied. So far, my observations point to the positive effect domain context has on reducing false positive PPI predictions.

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A Closed NPZ Model with Delayed Nutrient Recycling

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We consider a closed Nutrient-Phytoplankton-Zooplankton (NPZ) model that allows for a delay in the nutrient recycling. A delay-dependent conservation law allows us to quantify the total biomass in the system. With this, we can investigate how a planktonic ecosystem is affected by the quantity of biomass it contains and by the properties of the delay distribution. The quantity of biomass and the length of the delay play an significant role in determining the existence of equilibrium solutions, since a sufficiently small amount of biomass or a long enough delay can lead to the extinction of a species. Furthermore, the quantity of biomass and length of delay are important since a small change in either can change the stability of an equilibrium solution. We explore these effects for a variety of delay distributions using both analytical and numerical techniques, and verify results with simulations.

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Downscaling of regional climate scenarios within agricultural areas across Canada with a multi-variate, multi-site statistical model

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Crop yield forecasting and the integrated assessment of environmental and economic risks of agricultural production both require detailed information on historical and future impacts and variability of climate trends to reliably capture the broad spectrum of potential cumulative impacts of a changing global climate on soil, water and air quality. Regional dynamic climate model (RCM) output for historical re-analysis 1971-2000 and future scenario 2041-2070 periods is available for Canada (i.e., CGCM3-CRCM3 and HRM3-HadCM3 coupled models) from the North American Regional Climate Assessment Program (NARCCAP). The latest Canadian Regional Climate Model (CCCma-CanESM2) output is also available from Environment Canada for two Representative Concentration Pathways (RCP's) (RCP45 and RCP85) at a coarse scale (25-50 km). Typically, higher-resolution downscaled climate information (1-10 km, daily) is required by agroecosystem models and operational monitoring support systems to guide agricultural decision-making. Reliable methods are therefore needed to statistically downscale climate variability to agricultural ecosystem impact scales and to reduce uncertainty (bias and variance) in RCM model predictions. At the 10 km scale, changes in orography, large water bodies, land vegetation cover, and other evapotranspiration land-air feedbacks inact a strong regional-scale influence on seasonal changes in climate. Yet, downscaling models often rely on a single predictor variable and generate predictions at single sites without incorporating finer-scale physical influiences on climate that change the spatial covariance of precipitation, temperature and other climate variables. We present a multi-variate, multi-site method for downscaling climate to the 10 km scale for agricultural areas across Canada. This method employs variable-selection for a multivariate set of regional climate model predictors. Markov Chain Monte Carlo (MCMC) and k-NN (kth Nearest Neighbour Cluster) bootstrapping is employed to capture spatial covariance and temporal-lag dependence in climate predictors. We evaluate the performance of this model for a broad set of agricultural regions/climate zones across Canada. We outline several model improvements to better handle the large complex data inputs and address other computational issues. Our method may offer a rapid (automated) and reliable (cross-validated) way to generate high-resolution climate surfaces across Canada for use in agricultural decision-making.

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Parallel numerical methods for time dependent Schrodinger equations in the analysis of quantum heterostructures

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The growing demand for quantum dynamical simulations in the scientific and industrial applications requires the development of efficient numerical methods for the solution of time-dependent Schrödinger equation.

We present a new fully discretized numerical method for the solution of time-dependent Schrödinger equation with multi-band Hamiltonians obtained via the application of envelope function approximation to heterostructures composed from crystalline materials [2]. A solution $\Psi(t)$ of the following Cauchy problem for Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} - (H+V)\Psi = 0, \quad \Psi(0) = \Psi_0, \tag{1}$$

with H being a Hamiltonian (self-adjoint elliptic operator with semi-bounded spectrum) of the system defined in a heterostructure geometry Ω and V represents some potential field, can be formally represented as follows

$$\Psi(t) = e^{-itH}\Psi_0 + \int_0^t e^{-i(t-s)H}V(s)ds, \tag{2}$$

provided that the initial state Ψ_0 is admissible. In order to derive the numerical method we apply the Dunford-Cauchy formula to the propagator e^{-itH} from (2) and then approximate the resulting infinite integrals by efficient numerical quadrature rule, similar to the one used in [3]. By tailoring the parameters of the contour from Dunford-Cauchy formula to the spectral properties of operator $H+V$ the approximation of (2) is reduced to the series of independent stationary Schrödinger equations in the form of the following boundary value problem (BVP)

$$(z_k I - H)\Phi = V_k, \quad \Phi|_{\partial\Omega} = 0,$$

where V_k are functions dependent on the potential V and the initial state Ψ_0 and z_k is a set of points belonging to the contour of integration. Those series of BVP's are solved concurrently with the help of parallel FEM package Deal.II [1]. Such an approach allows us to obtain two level of parallelism in computation. We also give a technique how to adjust the accuracy of FEM solver to the accuracy of the time-domain approximation.

To show the method's numerical efficiency we present several 2D and 3D examples for quantum dot heterostructures with spherical geometry.

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Invariant Solutions of the $2+1$ dimensional Gross-Neveu Equations

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We apply Lie and nonclassical symmetry methods to partial differential equations in order to derive solutions of the Gross-Neveu model in $d=(2+1)$ space-time dimensions. Nonclassical symmetries are determined and used to derive new solutions for the Gross-Neveu model. Finally, steps are taken to facilitate the incorporation of boundary conditions.

We utilize of a computer algebra system, SADE [1], to obtain symmetry generators and classical solutions to the Gross-Neveu equations in 2 and 3 space-time dimensions, namely

$$\left(i\gamma^{\mu}\partial_{\mu}-\lambda\left(\overline{\Psi}\Psi\right)\right)\Psi=0, \tag{1}$$

where Ψ is a spinorial variable in 2 or 3 space time dimensionsand the γ matrices are given by

$$\begin{aligned}\gamma^{\mu}_{(2)} &= \left(\sigma^{2},i\sigma^{1}\right),\\ \gamma^{\mu}_{(3)} &= \left(\sigma^{2},i\sigma^{1},i\sigma^{3}\right).\end{aligned}$$

Non-classical symmetries, are used to obtain not yet known solutions to this spinor model in the specific case of $2+1$ dimensions.

The method used to simplify and solve the determining system for nonclassical symmetries will be outlined, and a choice of ansatz will be justified in this case. The resulting symmetry generators will be utilized to obtain invariant solutions. Remarks about ways to incorporate boundary conditions into this specific case will also be made.

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Application of Advanced Diagonalization Methods to Quantum Spin Systems

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Quantum spin models play an important role in theoretical condensed matter physics and quantum information theory. One numerical technique that is frequently used in studies of quantum spin systems is exact diagonalization (see for example Ref. [1]). In this approach, numerical methods are used to find the lowest eigenvalues and associated eigenvectors of the Hamilton matrix of the quantum system. The computational problem is thus to determine the lowest eigenpairs of an extremely large, sparse matrix.

Although many sophisticated iterative techniques for the determination of a small number of lowest eigenpairs can be found in the literature, most exact diagonalization studies of quantum spin systems have employed the Lanczos algorithm. In contrast to this, other methods have been applied very successfully to the similar problem of electronic structure calculations. The well known VASP code for example uses a block Davidson method as well as the residual-minimization – direct inversion of the iterative subspace algorithm (RMM-DIIS) [2]. The RMM-DIIS method can however not be used with random start vectors. In order to obtain reliable results one of the other methods must be employed during the first iterations.

The Davidson algorithm is closely related to the Lanczos method but usually needs less iterations. The RMM-DIIS method was originally proposed by Pulay [3] and later modified by Wood and Zunger [4]. The RMM-DIIS method is particularly interesting if more than one eigenpair is sought since it does not require orthogonalization of the trial vectors at each step.

In this work we study the efficiency of the Lanczos, Block Davidson and RMM-DIIS method when applied to basic quantum spin models like the spin-1/2 Heisenberg chain, ladder and dimerized ladder. We have implemented all three methods and are currently applying the methods to the different models. In our presentation we will compare the three algorithms based on the number of iterations to achieve convergence and the required computational time

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Random Jitter Methods for Type 2 Ties in Survival Analysis

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In a survival data set with discrete time-varying covariates, it is common to encounter ties between event times and the times that the discrete time-varying covariates change. We refer to these types of ties as Type 2 ties. It has been found that the default method for Type 2 ties in current statistical software for the Cox proportional hazards (CoxPH) model may introduce bias to the estimation of model parameters [1]. We proposed a Random Jitter method to deal with Type 2 ties in the CoxPH model [1]. We investigate a Multiple Random Jitter method as a potential improvement of the previously proposed Random Jitter method.

In the Random Jitter method, we allow the time that the time-varying covariate changes to occur randomly just before or just after the tied failure time, so that the Type 2 ties are broken while the original ordering of the untied jump and event times is retained. The coefficient estimate and corresponding standard error estimate are obtained by analyzing the modified data set with standard statistical software.

In the Multiple Random Jitter method, the Random Jitter method is applied to the same sample m times and the results from each of the m jittered samples are combined. We present results of a simulation study which shows that the Random Jitter method performs as well as the Multiple Random Jitter method. The methods are illustrated using a real data set.

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