# AMMCS 2017

## INTERNATIONAL CONFERENCE

## AUGUST 20–25

### WATERLOO, ONTARIO, CANADA

# BOOK OF ABSTRACTS

General Chairs

Marc Kilgour

Roderick Melnik

Interdisciplinary AMMCS Conference Series

# The AMMCS 2017 Conference

# Book of Abstracts

Waterloo, Ontario, Canada

August 20–25, 2017

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| SS-ASQE | Analogue Signals in Quantum Environments: The Physics and Mathematics of Propagation and Control |
| SS-CC | Computational Chemistry |
| SS-CDAHS | Complex Data Analysis in Health Science |
| SS-CNT | Computational Number Theory |
| SS-DAG | Dynamics and Games |
| SS-DASO | Data Analytics for System Optimization |
| SS-DETA | Delay Equations: Theory and Applications |
| SS-FCA | Fractional Calculus and Applications |
| SS-FD | Fair Decisions |
| SS-GLS | Geocomputational Landscapes and Spaces |
| SS-GMCTA | Geometric Mechanics and Control: From Theory to Applications |
| SS-IM | Industrial Mathematics |
| SS-MFMCR | Mathematical Finance — Modeling, Computation and Risk Management |
| SS-MMNN | Mathematical Models for Nanoscience and Nanotechnology |
| SS-MSED | Modelling of Socio-Economic Dynamics |
| SS-NDSA | Nonlinear Dynamical Systems and Applications |
| SS-OCDG | Optimal Control and Differential Games |
| SS-RAWP | Recent Advances in Mathematical and Computational Aspects of Wave Propagation |
| SS-RPNMSC | Recent Progress in Numerical Methods and Scientific Computing |
| SS-SMCGPL | Symbolic Methods in Code Generation and Programming Languages |
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| CODE | TITLE |
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| CS-APMRE | Applied Problems and Methods in Research & Education |
| CS-BSM | Mathematics and Computation in Biological Sciences and Medicine |
| CS-CACO | Computational Algebra, Combinatorics and Optimization |
| CS-CPC | Computational Physics and Chemistry |
| CS-DSDE | Applications of Dynamical Systems and Differential Equations |
| CS-ENV | Mathematical Modelling in Environmental Sciences and Models for Complex Media |
| CS-FINANCE | Financial Mathematics and Computation |
| CS-MECHE | Computational Mechanics and Engineering |
| CS-MODELING | Partial Differential and Integral Equations in Mathematical Modeling |
| CS-POST | AMMCS-2017 Poster Session |

# Lectures

# Plenary Lectures

# Learning from Elastic Network Models: From Proteins to Chromatin Dynamics

## Ivet Bahar, University of Pittsburgh

**Abstract:** Elastic network models proved to be powerful tools for exploring the collective dynamics of biomolecular systems in the last two decades. Numerous examples demonstrate their applicability to a broad range of phenomena, from allosteric transitions, to modeling protein-substrate interactions key to regulation and signaling events, to supramolecular machinery. Recent advances in cryo-EM characterizaton of big structures as well as genome-scale identification of 3D contacts between gene loci now open the way to a new level of applications, including the exploration of the 3D structural dynamics of the chromosomes, with the help of elastic network models, further supporting their utility as a tool applicable across multiple scales, from molecules to genome-wide associations.

## About the Speaker:

Ivet Bahar is currently Distinguished Professor and the Founding Chair of the Department of Computational and Systems Biology at the University of Pittsburgh, School of Medicine, and Associate Director of the U of Pittsburgh Drug Discovery Institute. She co-founded the first PhD degree-granting program between Carnegie Mellon University and the University of Pittsburgh, selected by the Howard Hughes Medical Institute and the National Institutes of Health as one of 10 national programs to offer interdisciplinary training at the interface between biological, physical and computational sciences. Dr. Bahar is a leader in theoretical and computational biophysics of protein dynamics, and multiscale modeling of complex biological systems and processes. She is known for her pioneering work on the development and application of elastic network models toward elucidating the structural dynamics of large biomolecular systems. Her studies have highlighted the significance of structure-encoded fluctuations in enabling functional interactions. She is an elected member of the European Molecular Biology Organization (EMBO). She has more than 250 publications in scientific journals, with $>$ 17,000 citations and an H-index of 66.

# Moral Artificial Intelligence and the Societal Tradeoffs Problem

**Vincent Conitzer, Duke University**

**Abstract:** AI systems increasingly need to make decisions with a moral component. Should a self-driving car prioritize the safety of its passengers over that of others, and to what extent? Should an algorithm that decides which donors and patients to match in a kidney exchange take features such as the patients age into account, and to what extent? I will briefly discuss two approaches to these problems: extending game-theoretic frameworks, and learning from examples of human decisions.

Under the second approach, we will generally find that not all humans agree! How, then, should we aggregate their judgments to make coherent decisions? This is a problem in computational social choice. I will present our work on the societal tradeoffs problem in which, based on multiple human judgments, we aim to find a specific value for $x$ in statements such as using one gallon of gasoline is as bad as creating $x$ bags of landfill trash.

The first part is joint work with Walter Sinnott-Armstrong, Jana Schaich Borg, Yuan Deng, and Max Kramer, and the second part with Rupert Freeman, Markus Brill, and Yuqian Li.

## About the Speaker:

Vincent Conitzer is the Kimberly J. Jenkins University Professor of New Technologies and Professor of Computer Science, Professor of Economics, and Professor of Philosophy at Duke University. He received Ph.D. (2006) and M.S. (2003) degrees in Computer Science from Carnegie Mellon University, and an A.B. (2001) degree in Applied Mathematics from Harvard University. Most of his research is on artificial intelligence (especially multiagent systems) and economic theory (especially game theory, social choice, and mechanism design). Conitzer has received the Social Choice and Welfare Prize, a Presidential Early Career Award for Scientists and Engineers (PECASE), the IJCAI Computers and Thought Award, an NSF CAREER award, the inaugural Victor Lesser dissertation award, an honorable mention for the ACM dissertation award, and several awards for papers and service at the AAAI and AAMAS conferences. He has also been named a Guggenheim Fellow, a Kavli Fellow, a Bass Fellow, a Sloan Fellow, and one of AIs Ten to Watch. Conitzer and Preston McAfee are the founding Editors-in-Chief of the ACM Transactions on Economics and Computation (TEAC).

# The Mathematical Limits of Sensory Integration and Control

**André Longtin, University of Ottawa**

**Abstract:** Theoretical studies of brain function have led to advances in a number of areas of applied mathematics. Recent advances are highlighted here in the context of sensory systems. These systems provide a particularly good window onto questions of neural dynamics, control and information processing, because they have a well-characterized physical input. This talk will first present recent work on information processing at the limits of sensory detection. The probabilistic encoding of sensory signals as modulations of intrinsically correlated neural point processes is shown to enhance their detectability and information content as sequences of firing or "spike" times. Downstream neurons further aim to derive optimal information about the position of objects in the environment. Their sensitivity is found to peak at a characteristic distance where the Fisher information is maximized. This result relies on a correction to the Fisher information for the positive correlations observed in the stochastic firing patterns. It provides a first mathematical description of a sensory focus, and this focal point corresponds to the transition from periodic to chaotic dynamics. Finally we discuss a stochastic optimal control problem to precisely target the spike times of a leaky integrate-and-fire (LIF) model of a neuron with noise. Such a model is in fact an Ornstein–Uhlenbeck process with an absorbing boundary, for which we are controlling the mean first passage time. The optimal control problem is solved using dynamic programming when the controller has access to the voltage (closed-loop control), and using a maximum principle for the transition density when the controller only has access to the spike times (open-loop control).

## About the Speaker:

André Longtin is the University Research Chair in Neurophysics at the University of Ottawa, as well as Chairman of its Physics Department. He runs the Neurophysics and Nonlinear Dynamics Group, working at the interface of physics, applied mathematics, biology and medicine. His main interests lie in theoretical and computational neuroscience and the interaction of deterministic systems with noise. He received an honours B.Sc. Physics in 1983 and M.Sc. Physics in 1985 from the Université de Montréal, and his Ph.D. in Physics from McGill University in 1989. He joined Los Alamos National Laboratory as an NSERC Postdoctoral Fellow and a Los Alamos Directors Funded Fellow, where he held a joint position in the Theoretical Division T13 (Complex Systems) and the Center for Nonlinear Studies. He began as assistant professor of Physics in 1992 at the University of Ottawa. He is Professor since 2002, and cross-appointed to the Departments of Cellular and Molecular Medicine and of Mathematics and Statistics. He is founding co-director of the University of Ottawa Center for Neural Dynamics and a Fellow of the American Physical Society. He sits on the editorial board of Biological Cybernetics, Cognitive Neurodynamics, Bulletin of Mathematical Biology, Journal of Mathematical Neuroscience and Frontiers in Computational Neuroscience. He was awarded a Premiers Research Award in 1999, the inaugural award for Interdisciplinary research at U. Ottawa in 2004 (with Len Maler), a senior Humboldt Research Prize in 2010, and the NSERC Brockhouse Canada Prize in Interdisciplinary Research with Len Maler in 2017 for uncovering key features of the neural code.

# Scaling Limits of Stochastic Networks

**Kavita Ramanan, Brown University**

**Abstract:** Stochastic networks arise in a variety of applications, ranging from communication and service networks to biochemical reaction networks. In many cases, these networks are too complex to be amenable to an exact analysis, and so it is useful to identify tractable approximations that provide qualitative insight into the dynamics, and whose accuracy can be rigorously justified via limit theorems in a suitable asymptotic regime. This talk will provide a survey of mathematical methods that have been developed to identify and analyze these scaling limits in different settings, and the qualitative insight they provide into network performance and design. We will also provide some illustrative examples of how the mathematical tools developed to analyze stochastic networks have been applied in other areas of probability, for the study of interacting particle systems, random matrices, and models in math finance.

## About the Speaker:

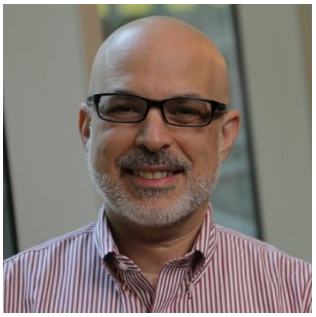
Kavita Ramanan is a professor at the Division of Applied Mathematics at Brown University. She previously held positions as professor of mathematics at Carnegie Mellon University and a Member of Technical Staff at Bell Laboratories. Her research lies in the area of probability theory, stochastic processes and their applications, including stochastic analysis, high-dimensional probability, large deviations, and applications to stochastic networks. She was awarded the Erlang Prize for outstanding contributions to applied probability by the INFORMS Applied Probability Society in 2006, was elected a fellow of the IMS (Institute for Mathematics and Statistics) in 2013 and was awarded the IMS Medallion in 2015. She has served on the editorial boards of several journals, including the Annals of Probability, Annals of Applied Probability, Queueing Systems and Stochastic Analysis and Applications, and is currently the Area Editor of Mathematics of Operations Research. She is the faculty founder of the AWM student chapter at Brown University and also runs a math outreach group at Brown called the Math CoOp.

# Big Data's Dirty Secret

**Harvey Stein, Bloomberg LP and Columbia University**

**Abstract:** "Let the data speak for themselves." "We apply machine learning to the problem of..." These are two commonly heard phrases these days. But what data exactly are we speaking about, and what do we intend to do with it? What is ignored all too often is the quality of the data being used and how it impacts the analyses being done. Are there holes in the data? Are there anomalies? Given how dirty data can be, a more apt phrase might be "Garbage in, garbage out." In this talk we will discuss some of the data problems we've encountered in financial data, and approaches that can be used to address them. Our particular focus will be on techniques we've employed to deal with missing data and bad data in credit default swap (CDS) spread histories.

## About the Speaker:



Harvey J. Stein is Head of the Quantitative Risk Analytics Group at Bloomberg, responsible for all quantitative aspects of Bloomberg's risk analysis products. Dr. Stein is well known in the industry, having published and lectured on mortgage backed security valuation, CVA calculations, interest rate and FX modeling, credit exposure calculations, financial regulation, and other subjects. Dr. Stein is also a member of the board of directors of the IAQF, an adjunct professor at Columbia University, a board member of the Rutgers University Mathematical Finance program and of the NYU Enterprise Learning program, and organizer of the IAQF/Thalesians financial seminar series. He received his BA in mathematics from WPI in 1982 and his PhD in mathematics from UC Berkeley in 1991.

# A Polytopal Generalization of Sperner's Lemma

**Francis Edward Su, Harvey Mudd College**

**Abstract:** Sperner's lemma is a statement about labelled triangulations of simplices whose applications include: finding fixed points of highly nonlinear functions, and computing Nash equilibria in game theory. With J. DeLoera and E. Peterson, we prove a polytopal generalization of Sperner's lemma to polytopes in two different ways, one constructive and one non-constructive, and give applications of this result: to cake-cutting problems, to minimal triangulations of polytopes, and to the game of Hex.

## About the Speaker:

Francis Edward Su is the Benediktsson–Karwa Professor of Mathematics at Harvey Mudd College, and Past-President of the Mathematical Association of America. He received his Ph.D. from Harvard University under Persi Diaconis. He will be Chern Professor at MSRI during Fall 2017, co-organizing a semester on Geometric and Topological Combinatorics. His research is in this area, with a focus on applications to the social sciences, and he has received multiple NSF research grants for his work. He serves as an Associate Editor for the SIAM Journal on Discrete Mathematics. He also has a passion for teaching and popularizing mathematics. From the Mathematical Association of America, he received the 2001 Hasse Prize for expository writing, and the 2013 Haimo Award for distinguished teaching. He authors the popular Math Fun Facts website and is creator of "MathFeed," the math news app.

# Mathematical and Computational Modeling of Epidemics Does More Than Forecast

**Alessandro Vespignani, Northeastern University**

**Abstract:** Recent years have witnessed the development of data driven models of infectious diseases rooted in the combination of large-scale data mining techniques, computational approaches and mathematical modeling. Although these models are increasingly used to support public-health decisions they are often under debate by only considering their value as forecasting tools. Here I will discuss, by using specific modeling examples of the H1N1 pandemic and the West Africa Ebola epidemic, how computational models can be used in real time to provide situational awareness, intervention planning and projections, and the identification of factors that fundamentally influence the course of an outbreak.

## About the Speaker:

Prof. Vespignani received his undergraduate degree and Ph.D., both in physics and both from the University of Rome "La Sapienza," in 1990 and 1994 respectively. He completed his postdoctoral research at Yale University and Leiden University. Prof. Vespignani worked at the International Center for Theoretical Physics (UNESCO) in Trieste and at the University of Paris-Sud in France as a member of the National Council for Scientific Research (CNRS) before moving to Indiana University in 2004. Before joining Northeastern University Vespignani was J.H.Rudy Professor of Informatics and Computing at Indiana University and serving as the Director of the Center for Complex Networks and Systems Research and the Associate Director of the Pervasive Technology Institute. Vespignani is elected fellow of the American Physical Society, member of the Academy of Europe, and fellow of the Institute for Quantitative Social Sciences at Harvard University. He is serving in the board/leadership of a variety of professional association and journals and the Institute for Scientific Interchange Foundation.

# Gaussian Processes and the Statistical Analysis of Computer Experiments

**William Welch, University of British Columbia**

**Abstract:** The presentation will be in three parts: the history, the current use, and the future of Gaussian processes (GPs) in the statistical analysis of computer models.

Why are GPs popular for computer experiments? Over the last quarter century GPs have become widespread in statistical, engineering, and other disciplines for the analysis of computer models. Their popularity probably stems from three major advantages: (1) they adapt to nonlinear input-output relationships in a data-adaptive way; (2) they may require relatively few runs of the computer model (important if the computer code is computationally demanding) and (3) they provide a measure of prediction uncertainty that is often realistic even when modelling a deterministic function. These basic properties will be reviewed.

How are GPs used to achieve scientific and engineering objectives? Computer experiments are carried out with one or more of many purposes in mind: sensitivity analysis, calibration of unknown parameters, optimization, propagation of input uncertainty to statistical properties of the output, and so on. A broad overview of how GPs serve these goals will be given.

What about really complex phenomena? The sample size, i.e., number of computer-model evaluations, for decent prediction accuracy can be impractically large for some high-dimensional, complex computer codes and even for toy problems. Some recent work to adapt GPs to expand the functions that can be usefully modelled will be briefly described.

## About the Speaker:

Will Welch joined the Department of Statistics, UBC as a Professor in 2003 and was Head of Department from 2003 until 2008. Prior to that he was at the University of Waterloo for 16 years. He also holds the honorary title of Visiting Professor in the Business School, Loughborough University, UK.

Welch's research spans computer-aided design of experiments, quality improvement, the design and analysis of computer experiments, statistical methods for drug discovery, and machine/statistical learning. The work is highly cited: please see Google Scholar. In 2000 he won the American Statistical Associations Statistics in Chemistry Prize.

Welch has served on the editorial boards of the Annals of Applied Statistics, the Canadian Journal of Statistics, and the Journal of Uncertainty Quantification. He has also served as Associate Director of the Canadian Statistical Sciences Institute (CANSSI).

# Adaptive Enriched Galerkin Methods for Miscible Displacement in Porous Media

## Mary Wheeler, University of Texas at Austin

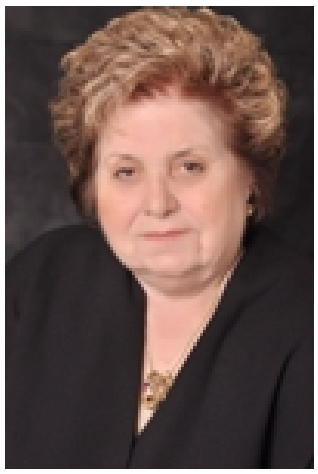
**Abstract:** Miscible displacement of one fluid by another in a porous medium has attracted considerable attention in subsurface modeling with emphasis on enhanced oil recovery applications. Here flow instabilities arising when a fluid with higher mobility displaces another fluid with lower mobility is referred to as viscous fingering. The latter has been the topic of major physical and mathematical studies for over half a century. Recently, viscous fingering has been applied for proppant-filled hydraulic fracture propagation to efficiently transport the proppant to the tip of fractures. The governing mathematical system that represents the displacement of the fluid mixtures consists of pressure, velocity, and concentration.

Here we present a novel approach to the simulation of miscible displacement by employing an adaptive enriched Galerkin finite element methods (EG) coupled with entropy residual stabilization for transport. EG is formulated by enriching the conforming continuous Galerkin finite element method (CG) with piecewise constant functions. EG provides locally and globally conservative fluxes, which is crucial for coupled flow and transport problems. Moreover, EG has fewer degrees of freedom in comparison with discontinuous Galerkin (DG) and an efficient flow solver has been derived which allows for higher order schemes. We have shown theoretically and computationally that a robust preconditioner can be achieved if one adds pre- and post smoothings to a block preconditioner involving CG and jumps in the discontinuous piecewise constants. Dynamic adaptive mesh refinement is applied in treating geological material discontinuities.

An additional advantage of EG is that only those subdomains that require local conservation need to be enriched with a treatment of high order non-matching grids. Our high order EG transport system is coupled with an entropy viscosity residual stabilization method introduced in to avoid spurious oscillations near shocks. Instead of using limiters and non-oscillatory reconstructions, this method employs the local residual of an entropy equation to construct the numerical diusion, which is added as a nonlinear dissipation to the numerical discretization of the system. The amount of numerical diffusion added is proportional to the computed entropy residual. This technique is independent of mesh and order of approximation and has been shown to be efficient and stable in solving many physical problems with CG. Finally we note that it is crucial to have dynamic mesh adaptivity in order to reduce computational costs for large-scale three dimensional applications; both for flow and transport. We employ the entropy residual for dynamic adaptive mesh renement to capture the moving interface between the miscible uids. It Our computational results indicate that the entropy residual can be used as a efficient posteriori error indicator.

This is joint work with Sanghyun Lee and Young-Ju Lee (University of Texas at Austin).

## About the Speaker:



About the speaker: Mary Fanett Wheeler is well-known researcher in computational science. She has been a member of the faculty at The University of Texas at Austin since 1995 and holds the Ernest and Virginia Cockrell Chair in the departments of Aerospace Engineering and Engineering Mechanics, and Petroleum and Geosystems Engineering. She is also director of the Center for Subsurface Modeling (CSM) at the Institute for Computational Engineering and Sciences (ICES). Before joining the faculty at UT Austin, Dr. Wheeler was the Noah Harding Professor in engineering at Rice University in Houston. Dr. Wheelers research interests involve numerical solution of partial differential systems with application to the modeling of subsurface flows and parallel computation. Applications of her research include multiphase flow and geomechanics in fractured porous media, contaminant transport in groundwater, and sequestration of carbon in geological formations. Dr. Wheeler has published more than 300 technical papers and edited seven books; she is currently an editor of five technical journals. Dr. Wheeler is a member of the Society of Industrial and Applied Mathematics and the Society of Petroleum Engineers. She is a Fellow of the International Association for Computational Mechanics and is a certified Professional Engineer in the State of Texas. She was co-organizer of the SIAM Activity Group in the Geosciences, and with Dr. Hans van Duijn, started the Journal on Computational Geosciences. Dr. Wheeler has received numerous honours and awards during her career; we list several recent honours. In February 2013, Dr. Wheeler was selected to receive the Lifetime Achievement Award of the International Society for Porous Media, InterPore. The award is given in recognition of her achievements in the area of subsurface flow and contaminant transport, and in recognition of her great contribution in increasing the visibility, credibility and prestige of porous media research. In May 2013, Dr. Wheeler received the John von Neumann Medal award from the Unites States Association for Computational Mechanics (USACM). It is the highest award given by USACM to honor individuals who have made outstanding, sustained contributions in the field of computational mechanics over substantial portions of their professional careers. In 2014, she was named an SPE honorary member, the organizations highest honor.

# Semi-Plenary Lectures

# Birkhoff normal form for nonlinear wave equations

**Walter L. Craig, McMaster University**

**Abstract:** Many theorems on global existence of small amplitude solutions of nonlinear wave equations in $\mathbb{R}^n$ depend upon a competition between the time decay of solutions and the degree of the nonlinearity. Decay estimates are more effective when inessential nonlinear terms are able to be removed through a well-chosen transformation. Additionally, most physically relevant wave equations can be formulated as Hamiltonian PDEs, and the analysis of their solutions can be considered in this context. In this talk, we construct Birkhoff normal forms transformations for the class of wave equations which are Hamiltonian PDEs and null forms, using the flow of an auxiliary Hamiltonian system . This gives a new proof via canonical transformations of the global existence theorems for null form wave equations of S. Klainerman and J. Shatah in space dimensions $n \geq 3$. The case $n = 2$ is also under consideration, which involves a normal forms interpretation of modified scattering. These results are work-in-progress with A. French and C.-R. Yang.

## About the Speaker:

Walter L. Craig is a Canadian mathematician, currently a Canada Research Chair in Mathematical Analysis and Applications at McMaster University. Craig earned his Ph.D. from New York University in 1981; his dissertation, A Bifurcation Theory for Periodic Dissipative Wave Equations, was supervised by Louis Nirenberg. In 2012, he became one of the inaugural Fellows of the American Mathematical Society.

# Computing Zeta Functions in Average Polynomial Time

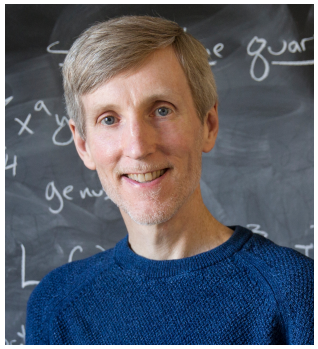
**Andrew Sutherland, MIT**

**Abstract:** Let $X$ be a smooth projective curve defined over a finite field of prime order p. Determining the number of rational points on $X$, or more generally, computing the zeta function of $X$, is a core problem in computational number theory with many applications. For curves of genus $g = 1$, Schoof uses a CRT approach to obtain a polynomial-time algorithm; Schoof's algorithm has been generalized to curves of higher genus by Pila, with a running time that is polynomial in log p but exponential in $g$. Alternatively, $p$-adic approaches based on generalizations of Kedlaya's algorithm yield a running time that is polynomial in $g$ but exponential in $\log p$. No algorithm with a running time that is polynomial in both $g$ and $\log p$ is currently known.

Now suppose $X$ is instead defined over the rational numbers, and consider the sequence of curves $X_p$ obtained by taking the reductions of $X$ modulo primes $p$ of good reduction up to some bound $N$. The problem of computing the zeta functions of all the $X_p$ naturally arises when one wishes to compute the $L$-function of $X$, or to study its Sato–Tate distribution. Harvey has shown that this problem can be solved in time quasi-linear in $N$; the average time to compute the zeta function of each of the curves $X_p$ is polynomial in both $g$ and $\log p$.

I will report on practical implementations of this algorithm, focusing in particular on curves of genus 3, both hyperelliptic and non-hyperelliptic, where we have recently obtained results that are dramatically faster than using either a CRT or $p$-adic approach to compute the zeta function of each $X_p$ individually.

## About the Speaker:



Andrew Sutherland received his undergraduate degree in mathematics from MIT in 1990. Following a successful career as an entrepreneur in the software industry, he returned to MIT and completed his Ph.D. in 2007, winning the George M. Sprowles Prize for his thesis on order computations in generic groups. Sutherland is currently a Principal Research Scientist at MIT with a research focus in computational number theory and was recently awarded the Selfridge Prize for his work in this area. He has played a leading role in a number of large scale collaborations in open mathematics, including the polymath project on prime gaps and the $L$-functions and Modular Forms Database (LMFDB), and he serves on the editorial board of several journals, including Mathematics of Computation.

# AMMCS Prize-Winning Lecture

# Kolmogorov–Wiener Prize for Young Researchers Sparse Polynomial Approximation of High-dimensional Functions

**Ben Adcock, Simon Fraser University**

**Abstract:** Many problems in scientific computing require the approximation of smooth, high-dimensional functions from limited amounts of data. For instance, a common problem in uncertainty quantification involves identifying the parameter dependence of the output of a computational model. Complex physical systems require computational models with many parameters, resulting in multivariate functions of many variables. Although the amount of data may be large, the curse of dimensionality essentially prohibits collecting or processing enough data to reconstruct the unknown function using classical approximation techniques.

In this talk, I will give an overview of the approximation of smooth, high-dimensional functions by sparse polynomial expansions. I will focus on the recent application of techniques from compressed sensing to this problem, and demonstrate how such approaches theoretically overcome the curse of dimensionality. If time, I will also discuss a number of extensions, including dealing with corrupted and/or unstructured data, the effect of model error and incorporating additional information such as gradient data. I will also highlight several challenges and open problems.

This is joint work with Casie Bao, Simone Brugiapaglia and Yi Sui (SFU).

## About the Speaker:

Benjamin Adcock received his PhD from the University of Cambridge in 2010. After his graduation, he received NSERC and PIMS Postdoctoral Fellowships and was carrying his research at Simon Fraser University. In 2012 he joined Purdue University as an Assistant Professor. Since August 2014 he is on the faculty of mathematics at Simon Fraser University. Dr. Adcocks research interests include applied and computational harmonic analysis, sampling theory, compressed sensing, as well as approximation theory and numerical analysis. He made original significant contributions to sampling theory and compressed sensing which have potential applications in the areas ranging from medical imaging to geophysical signal processing. At the time of the award, he has published twenty journal publications, most of which are in the top tier journals of his field. Dr. Adcocks work bridges the gap between theory and practice by developing and applying highly innovative mathematical tools.

# Special Sessions

# SS-AAIP Applied Analysis and Inverse Problems

# Boundary data identification for an electromagnetic problem by means of the potential field method

Tong Kang
School of Sciences, Communication University of China,
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**Abstract.** We give this talk on a boundary data identification for an electromagnetic problem by means of the potential field method (the $\boldsymbol{A}$-$\phi$ method). One part of the boundary is over-determined. The other part of the boundary is unreachable and has to be determined as a part of the problem. We design a constructive algorithm by the $\boldsymbol{A}$-$\phi$ formulation to solve this problem. The numerical scheme is based on the steepest descent method (SDM) for the minimization of a regularized cost functional, having its derivative determined via an adjoint method. We analyse the properties of the cost functional and prove the convergence of the minimization process. The method is supported by several numerical experiments.

*Key words:* Maxwell's equations; Boundary data identification; $\boldsymbol{A}$-$\phi$ method; Steepest descent method; Convergence.

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# Circle Inversion Iterated Function Systems

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Suppose $C$ is a circle in $\mathbb{R}^2$ with radius $r > 0$ and center $o$. We can represent $x \in \mathbb{R}^2$ as $x = ar(\cos(\theta), \sin(\theta)) + o$, where $\theta$ is measured from any fixed ray originating from $o$ and $a \geq 0$. The circle inversion map $T$ with respect to $C$ is given by

$$T(x) = \frac{1}{a} r(\cos(\theta), \sin(\theta)) + o,$$

for $x \in \mathbb{R}^2 \setminus \{o\}$. Consider $N$ circles and $N$ associated circle inversion maps. In the literature the chaos game is played with these maps to generate pictures [1, 2].

In this work we establish rigorously that there exists an attractor to the iterated function system given by the circle inversion maps and that the chaos game will generate the attractor. We do this by proving that the IFS $\overline{T}$ given by certain compositions of modified, non-expansive circle inversion maps $T_i$, $i = 1, 2 \ldots N$, is contractive. We then prove that the attractor of $\overline{T}$ is the same as the attractor of the system of unmodified circle inversion maps and that the chaos game will generate the attractor if it is played with both the individual modified maps and individual unmodified maps.

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# Computational Resolution of the Inverse Problem of Kinetic Capillary Electrophoresis (KCE) to Arbitrary Accuracy

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The direct problem of efficiently generating accurate numerical solutions to a particular set of partial differential equations, has been resolved via a multimesh algorithm that fully overcomes the typical instability arising from the interaction of the diffusion and convection terms [2]. This potent solution to the direct problem allows the resolution of the inverse problem on a reasonable timescale. The inversion essentially entails the optimization of a non-linear error objective, computed between the experimental target signal and the signals generated numerically at each iteration [4, 3]. Estimating the starting point for the optimization, poses a challenge in itself [5]. Furthermore, control of the error in the sought parameters is demonstrated, enabling the resolution of this inverse problem to arbitrary accuracy for exact target signals.

This work has been implemented as a software package [1].

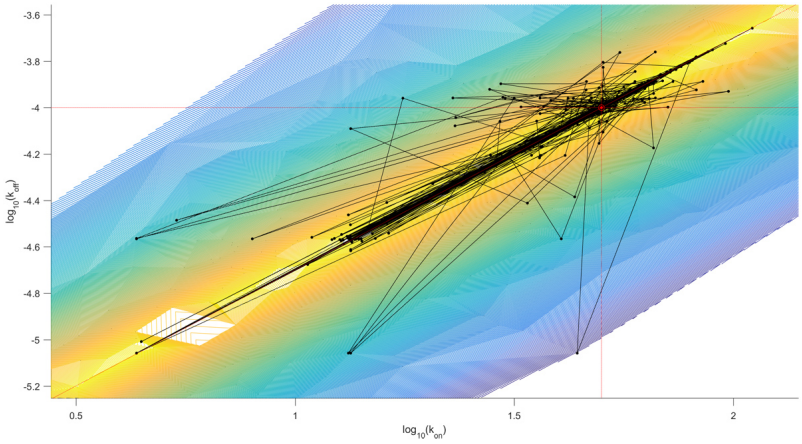


Figure 1: The Cuckoo Search algorithm minimizing the error target function.

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# Cubic zipper fractal interpolation function

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Fractal interpolation[1] is a modern technique to analyze various irregular data in nature and scientific experiments. If we choose the scaling factors appropriately, then the fractal function is $\mathscr{C}^2$-smooth in nature, but its second derivative is a typical non-smooth fractal[2]. This paper introduces a new type cubic spline fractal interpolation function (FIF) based on the concept of zipper that possesses a binary array known as signature. In particular, we have proposed a novel class of $\mathscr{C}^2$-cubic zipper FIFs using moments (2nd derivatives at the grid points), where every element of this class has two degrees of freedoms, namely: (i) vertical scaling factors $\{\alpha_i \in (-1,1) : i = 1,2,\ldots,N\}$ (ii) signatures $\{\varepsilon_i \in \{0,1\} : i = 1,2,\ldots,N\}$ for a prescribed interpolating data set $\{(x_i,y_i) : i = 0,1,\ldots,N\}$. The fractal cubic spline interpolant (the classical $\mathscr{C}^2$-cubic spline) is a particular case of the proposed cubic zipper FIFs when all signatures are zero (all $\alpha_i = 0$)[3]. The convergence results of cubic zipper FIF to the original function $\Phi(x) \in \mathscr{C}^r[x_0,x_N]$ are deduced for $r = 2,3,4$. The usefulness of cubic zipper FIF with various signatures and scaling factors are illustrated through examples.

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# Error Estimation for Fan Bea Algorithm

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Shannon theory is an exact method to recover a bandlimited signal from its sampled values in discrete implementation, using sinc interpolators. But sinc based results are not much satisfactory for bandlimited calculations so that convolution with window function, having compact support, has been introduced. Convolution Backprojection algorithm with window function is an approximation algorithm. In this paper, the error has been calculated, arises due to this approximation nature of reconstruction algorithm. This result will be defined for fan beam projection data which is faster than parallel beam projection. An approximation inversion formula by Radon transform is accomplished by filtered backprojection algorithm. Since projection data is continuous in nature, thus to reconstruct an image at any point requires projections data in all the directions and this increases the exposer of patient in CT machine. Fan beam technique provides a new geometry to calculate projection data, which is limited the scanning time because large number of rays are coming from single source.

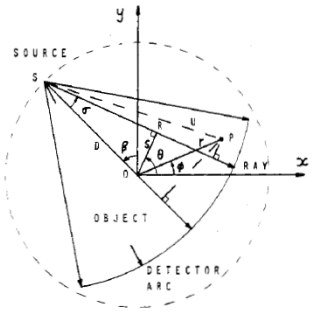


Fig. 1. Fan Beam Reconstruction Geometry

The approximation for Fan Beam geometry is given by

$$f_c\,(x,y) \;\simeq\; f \;*\; K_c\,(x,y)$$

where $K_c\,(x,y)$ is a filter function. As back-projection algorithm provides an approximation result for reconstruction of image function $f\,(x,y)$. In this script, an inherent error $E = \tilde{f} - f$ for fan beam geometry has been calculated.

$$E(x,y) = \frac{-1}{4\pi^2} W^{''}(0) \frac{\pi}{(bD)^2} \Delta^2 f \qquad (2)$$

This outcome for error in reconstruction algorithm provided that b and derivative value of window function (or filter function), we obtained better result by increasing distance between source and origin of object function. Similarly, for the smooth function and fix distance D we have convergence for larger band-limit value b.

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# Extending the Application of Colour Stealing for Contractive Iterated Function Systems

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A contraction mapping $f$ on a metric space $(X,d)$ satisfies the property that $d(f(x),f(y)) \leq kd(x,y)$ for all $x,y \in X$ with $k \in [0,1)$. Banach's fixed point theorem states that given a complete metric space $(X,d)$ and a contraction mapping $f$ satisfying $f : X \to X$, there exists a unique fixed point $\bar{x} \in X$ satisfying $f(\bar{x}) = \bar{x}$; further, this fixed point may be approximated with arbitrary precision by iterating $f$ upon any initial point in $X$.

Given a complete metric space $(X,d)$, a *contractive iterated function system* (IFS) is a union of such set-valued contraction mappings. An IFS is itself a contraction mapping on $(\mathscr{H}(X),d_h)$ where $\mathscr{H}(X)$ is the set of all compact subsets of $X$ and $d_h$ represents the Hausdorff metric. Given particular choices of mappings, the fixed point of an IFS, called an *attractor*, has the properties of a fractal and a graphical depiction which can be visually attractive. The attractor of an IFS is continuously dependent upon the parameters defining the IFS; small changes in these parameters result in only small changes in the attractor. Plotting IFS can be challenging and computationally intensive, so we employ a *random algorithm* referred to as the *chaos game*. Here, given a seed point, IFS mappings are chosen at random in sequence, with each subsequent point mapped from the one before it through the new mapping. Utilizing this approach, we may plot attractors accurately and quickly.

Attractors may be coloured in many ways, but of interest is the method of *colour stealing* [1, 2]. Given a random sequence of selected mappings, we plot points using the first IFS to draw the attractor, as usual. Simultaneously, we consider a different plot overlaid with a colourful image and a second IFS. The second IFS specifies a colour on this image each time a point is plotted using the first IFS; we use this colour to paint the point. Since a single point may be visited at many different times during the chaos game and thus be associated with many different colours, it is important to have a method of uniquely identifying a single colour to use. This issue is compounded in computer implementation, where many points fall into any single pixel, whose colour must be chosen. To solve this problem, the notion of *code space*, associated *code metric*, and the concept of the *fractal top* have been defined previously. Now, we introduce *finite code space* and a metric for use in practical computation. We extend the notion of the fractal top by defining a *fractal bottom* and showcase some resulting attractors. Finally, we combine these concepts with the concept of continuous dependence of attractors upon IFS parameters to produce families of IFS attractors, all coloured using the colour stealing technique.

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# Image-Driven Boundary Value Inverse Problems

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For the Sturm-Liouville two-point boundary value problem [1]

$$\begin{aligned}(k(x)u'(x))' + q(x)u(x) &= f(x)\\ u(a) &= u_a\\ u(b) &= u_b\end{aligned}$$

we consider the inverse problem:

*Given $f(x)$, $q(x)$, and a greyscale image of the level values of $u(x)$, recover an estimate of $k(x)$.*

For context, we can think of the greyscale image as representing the isotherms of the steady-state heat distribution, concentrations in a chemical system, or population densities. The collage method for treating boundary value inverse problems, given observational data values across the domain, is well-established in the literature [2, 3]. In our case, however, the image gives no actual values, but does give some comparative information across the domain. We consider several scenarios for which we can treat the inverse problem. We explore several examples to illustrate the method.

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# Investigation of Mannheimia haemolytica and Bovine Respiratory Disease towards generalized Immune Response through Mathematical Modelling

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Mannheimia haemolytica, formally known as Pasteurella haemolytica A1, is a vicious bacterial infection that causes fibronous pneumonia in the respiratory tract of cows. This bacterial infection is easily induced through weather, daily stressors and unfavourable environments all of common occurrence in a cow's daily routine. Without proper immunities or a developed mature immune system, as in calves, the infection travels down the respiratory tract of the cow and establishes itself in the lungs causing severe discomfort and build up of a fluid-like substance resulting most often in death. According to the USDA in a 2010 study, more than one million cattle are lost annually due to respiratory problems, representing approximately 30% of the total loss of cattle per year [2]. Current immunization strategies, such as vaccinations, have shown significant increase in immune response and defense from this infection, but timing and approaches to immunization are not fully understood.These statistics are expected to grow as demand and productivity increase, driving the motivation for the research and analysis of this problem. Our main goal is to mathematically model the immune response pathway and explore different immunization options.

We present and analyze a mathematical model created through the use of ordinary differential equations. The ODEs intend to replicate the biological process of the immune system and the interaction that occurs with bacterial infection. Important behaviours of the model are explored via simulation and numerical analysis. Numerical data of this infection, gathered by Dr. Doug Hodgins, is used to estimate parameter values in the model [1]. Our first goal of the model is to explore how to potentially maximize the natural immune response in cattle. A second goal of this model is to incorporate the addition of a current market safe vaccine. We present ideas on how to extend this model into a generalized respiratory immune response model.

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# Iterated function systems with place-dependent probabilities and the inverse problem of approximation of measures using moments

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We are concerned with the approximation of probability measures on a compact metric space $(X,d)$ by invariant measures of iterated function systems with place-dependent probabilities (IFSPDP): systems of contraction mappings on $X$, $\mathbf{w} = \{w_1, w_2, \cdots, w_N\}$, with associated probabilities $\mathbf{p} = \{p_1, p_2, \cdots, p_N\}$, the latter of which are place-dependent, i.e., $p_i : X \to \mathbb{R}$, as opposed to the constant probability case first examined in [2]. As such, $0 \le p_i(x) \le 1$, $1 \le i \le N$, and $\sum_{i=1}^N p_i(x) = 1$ for all $x \in X$. In this paper, we consider the special case $X = [0,1]$ with affine IFS maps and probabilities, i.e., $w_i = a_i x + b_i$, $p_i = \alpha_i x + \beta_i$, $1 \le i \le N$. The extension to $[0,1]^n$ is straightforward. Associated with an $N$-map IFSPDP is a "Markov" operator $M : \mathscr{M}(X) \to \mathscr{M}(X)$, where $\mathscr{M}(X)$ denotes the set of probability measures on (the $\sigma$-algebra of Borel subsets of) $X$. For any measurable set $S \subset X$, $d\nu(S) = d(M\mu)(S) = \sum_{i=1}^N (p_i \circ w_i^{-1}(S)) d(\mu \circ (w_i^{-1}(S))$ [3]. The main steps in our treatment are as follows:

1. The formal inverse problem of measure approximation may be posed as follows: Given a target measure $\nu \in \mathscr{M}(X)$, find an IFSPDP $(\mathbf{w}, \mathbf{p})$ with invariant measure $\bar{\mu}$ such that $d_{MK}(\bar{\mu}, \nu) < \varepsilon$, where $d_{MK}$ denotes the Monge-Kantorovich metric on $\mathscr{M}(X)$. We consider the following inverse problem: Given a target measure $\nu \in \mathscr{M}(X)$, find an IFSPDP $(\mathbf{w}, \mathbf{p})$ with associated (contractive) Markov operator $M : \mathscr{M}(X) \to \mathscr{M}(X)$ such that $d_{MK}(M\nu, \nu) < \delta$. From the "Collage Theorem" [1], a simple consequence of Banach's Fixed Point Theorem, $d_{MK}(\bar{\mu}, \nu) < \delta(1-c)^{-1}$, where $\bar{\mu}$ is the fixed point of $M$ and $c$ is its contractivity factor.

2. We perform the approximation by "moment matching." Let $D(X)$ be the set of all infinite moment vectors of measures $\mu \in \mathscr{M}(X)$, i.e., $D(X) = \{\mathbf{g} = (g_0, g_1, \cdots) \mid g_n = \int_X x^n \, d\mu \,, \ \mu \in \mathscr{M}(X)\}$. (Clearly, $g_0 = 1$.) Furthermore, define the following weighted $l_2$ metric on $D(X)$: $\bar{d}_2(\mathbf{g}, \mathbf{h}) = \left[\sum_{k=1}^\infty (g_k - h_k)^2 / k^2\right]^{1/2}$. Associated with the Markov operator $M$, there exists an operator $A : D(X) \to D(X)$ which is contractive in the metric $\bar{d}_2$. Using a "Collage Theorem for Moments" [2], we look for an IFSPDP such that $\bar{d}_2(A\mathbf{g}, \mathbf{g}) < \delta$, where $\mathbf{g}$ is the moment vector of the target measure $\nu$.

3. As in [2], we work with a fixed set of affine IFS maps $w_i, 1 \le i \le N$, and increase $N$ as necessary. The maps are selected from an infinite set of maps $\{w_i\}_{i=1}^\infty$ that satisfy an "$\varepsilon$-contractivity" refinement condition on $X$ [2]. For a given set of IFS maps $\mathbf{w}_N$, the minimization of the square of the moment collage distance, $\Delta_N = d_2(A_N\mathbf{g}, \mathbf{g})$, yields a quadratic programming (QP) problem in the unknowns $\alpha_i, \beta_i$, $1 \le i \le N$ which define the place-dependent probabilities, $p_i$. In the special case that we fix $\alpha_i = 0$, $1 \le i \le N$, the QP problem reduces to that for constant probabilities in [2]. Some examples and results of numerical computations will be presented.

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Numerical Solutions for an Extended Class of Boundary Value Problems

Abstract

In this paper, we present a new iterative scheme for solving a wide class of second and third order nonlinear boundary value problems that arise in various physical phenomena of applied and engineering sciences. The algorithm is based on embedding Green's functions into fixed point iterations including, Picard's and Krasnoselskii-Mann's schemes. Illustrative numerical examples are provided to demonstrate the efficiency, accuracy, effectiveness and simplicity of the proposed method in tackling such problems. A comparison of the results obtained by the proposed strategy with those resulting from the exact solutions and/or other existing methods reveals that the approach is highly accurate and converges fast.

**Keywords:** Second order nonlinear BVPs; Third order nonlinear BVPs; Green's functions; fixed point iterations

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# Numerical Stability of an integral equation applicable to the diagnosis of high-temperature plasma

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One of the most common high-temperature plasma diagnostics is to study the spectrum of bremsstrahlung X-ray wavelength range. For integral equation of the first kind, occurs when a restore operation of the electron energy distribution function (EEDF) in the spectrum of bremsstrahlung, obtained steady numerical solution using Tikhonov functional with a stabilizer of the second order. In this work, we consider the possibility of restoring of the EEDF when it deviates from the Maxwellian, which is important for the study of strongly unstable plasma [1].

In [2] under some assumptions and values of the parameter has defined concrete action of the experiment, we consider the integral equation relating the unknown distribution function of plasma electrons in the energy $f$ and bremsstrahlung spector $N$

$$\int_a^b H(E,\varepsilon)f(\varepsilon)d\varepsilon = N(\varepsilon), \qquad \varepsilon \in [a,b] \tag{1}$$

where the kernel $H$ - known continuous function. We write this equation in the form

$$Hf = N \tag{2}$$

In [2] an approximate solution of this integral equation in the case, when $||N - N^{\delta}|| = \delta$, it was proposed to look like extreme Tikhonov functional

$$M^{\alpha}[u] = ||Hu - N^{\delta}||^2 + \alpha||u'||^2$$

with the stabilizer of the first order $\alpha||u'||^2$. Extreme can be obtained as the solution of the Euler equation

$$\begin{aligned} H^*Hu - \alpha u'' &= H^*N^{\delta}, \\ u'(a) = 0 \quad , \quad & u'(b) = 0 \end{aligned}$$

The solution of this problem as an approximate solution (1) has a defect (including those with numerical implementation) «deformation» of the solution to the zero value of the derivative at the points $a$, $b$. To avoid this «effect», we propose to construct an approximate solution of the Euler equations for the Tikhonov functional with a stabilizer of the second order.

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# On oscillating integrals

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In this talk we will consider some inequalities of oscillating integrals. These integrals are available in many applications and their approximations is always sought. The unpredictability of their integrand fluctuations make it harder to predict their sign and predict their behavior. A concise mathematical approach will be given to explain their global behavior over a closed interval.

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# Population and Pollution Interactions in a Spatial Economic Model

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The topic of sustainable development has become very popular over the last decades, and both academics and policymakers are nowadays more interested than ever in understanding how to address the economy along a sustainable development path (Solow, 1974). Sustainability has been traditionally defined as the ability to satisfy *"the needs of the present without compromising the ability of future generations to meet their own needs"* (WCED, 1987). Thus, such a notion requires to carefully take into account the relation between population and environment. The channels through which human population affects the natural environment in which it lives and how in turn the environment may alter the evolution of human population have been long discussed in literature since Malthus' (1798) seminal work (see among others, Nerlove, 1991; Marsiglio, 2011). However, none of the existing works is able to relate the issue to geographical and spatial characteristics, since they all assume that the economy is simple a unique point in space and thus eventual heterogeneity are completely ruled out. This is clearly a strong simplification of reality and understanding the implications of geographical heterogeneity on the development process of a spatial-extended notion of economy is a very active and recent research topic, following Krugman's (1991) seminal work (see Camacho and Zou, 2004; Boucekkine et al., 2009; Xepapadeas, 2010). The goal of this paper is exactly to fill such a gap by analyzing the relation between population and environment from a spatial point of view, taking into account thus that the dynamics of population and the environment mutually affect each other not only over time but also across space. Our main results show that by neglecting the existence of spatial externalities the conclusions about the development process followed by specific locations in the entire spatial economy may be strongly misleading, suggesting thus that geographic heterogeneity and externalities may play an important role in the process of economic development.

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# Solving Inverse Problems for Fractional ODEs via the Collage Theorem

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Fractional Differential Equations have a number of real-world applications particularly in the disciplines of Engineering and Physics. Although far less prominent in the literature, these equations have the ability to explain a number of phenomenon more accurately than classical differential equations. In this talk we briefly introduce the idea of Fractional Calculus. We expand a few of the ideas from classical Calculus and use them to discuss an inverse problem for a general class of Fractional Ordinary Differential Equations (FODEs). With existence and uniqueness theory for classical ODEs as a guide, we use the collage theorem, a consequence of Banach's classical Fixed Point Theorem, to establish a "collage method" for solving such inverse problems under certain restrictions. We apply this method to some model FODEs in which we only use solution data (perhaps adding relative noise to simulate experimental error) to recover other parameters present in the model.

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# Solving Inverse Problems on a Perforated Domain via the Collage Method for Vector-valued Lax-Milgram Variational Problems

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The inverse problem literature is rich with problems considering the estimation of unknown parameters in a proposed governing model of a phenomenon of interest. Many such problems can be cast in terms the approximation of a target element in a complete metric space by the fixed point of a contraction map. A simple consequence of Banach's Fixed Point Theorem called the Collage Theorem can be employed to shift from the problem of directly minimizing the fixed point approximation error to instead minimizing a simpler quantity referred to as the "collage distance" (because of its roots in fractal imaging). This approach and general philosophy has been used to establish "generalized collage theorem"s in various settings. Very recently in [1], it was shown the vector-valued Lax-Milgram Theorem could be used to generate such a result useful for solving related inverse problems.

Other very recent work focuses on solving inverse problems on perforated domains [3]. The work establishes that the solution of the parameter estimation on a perforated domain can be approximated by instead solving the inverse problem on the much easier to work with associated solid domain.

In this work, we consider vector-valued variational problems on a perforated domain and show that the inverse problems on the perforated and associated solid domains can be similarly connected. Theory and examples will be presented.

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# Total Variation Denoising using Iterated Function Systems on Mappings

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In fractal image coding based on Generalized Fractal Transforms (GFT), one seeks to approximate a target image or signal by the fixed point of a contractive fractal transform operator (see [3] and the references therein).

The usual formulation involves a fixed set of geometric contraction maps along with a corresponding set of greyscale maps. The inverse problem, which involves the determination of the best greyscale map parameters for a given target image, is based on the so-called "Collage Theorem," a simple consequence of Banach's fixed point theorem.

In [2], the authors showed that one can find an iterated function system with greyscale maps (IFSM) to approximate any target signal or image with arbitrary precision, and they provided a suboptimal but systematic approach for doing so.

In [4] the authors extend the approach developed in [2] along two different directions: first they search for a set of mappings and greyscale map parameters that not only minimizes the collage error but also maximizes the entropy of the parameter set and, second, they try to maximize the sparsity of the set of greyscale parameters. In their formulation, the minimization of the collage error is studied as a multi-criteria problem.

In [5] the authors show that under certain hypotheses, an IFSM is a contraction on the complete space of functions of bounded variation (BV). It then possesses a unique attractor of BV. The authors also present some BV-based inverse problems based on the Collage Theorem for contraction maps.

The notions of total variation (TV) or bounded variation (BV) have had several applications in image analysis and, in particular, in noise removal. The main justification of this comes from the fact signals with spurious detail have high total variation. The process of reducing the total variation of the signal removes unwanted detail whilst preserving important details such as edges.

In this paper, we examine the idea of TV-based denoising applied to the inverse problem for Iterated Function Systems on Mappings. Numerical experiments show how the method works practically.

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# Stochastic Dynamic Multiple Objective Optimization with Application to Financial Portfolio Management

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A Calculus of Variations or an Optimal Control problem consists of identifying a feasible scheme, policy, program, strategy, or campaign, that allows to reach the optimal possible outcome of a system. From a mathematical point of view, it deals with the maximization or minimization of an objective functional that is often expressed as definite integral depending on state and/or control variables, and a set of constraints that describes the evolution of the underlying system. The mathematical model is formulated, for example, as systems of ordinary, partial, or stochastic differential equations or discrete dynamical systems, for both scalar and multi-objective decision making contexts. The most popular solution techniques used for solving the above problems are the Euler equation and the Hamilton Jacobi-Bellman equation. Nowdays these have become very active research areas with numerous contributions to the theory, in both deterministic and stochastic contexts. Its application to diverse fields such as biology, economics, ecology, finance, and management cannot be overlooked. The aim of this paper is twofold: first, to extend the definition of stochastic multiple objective model and the notion of stochastic Pareto efficient solution to the case of functionals defined on an abstract space. Second, to apply these extensions to the analysis of a class of stochastic dynamic multiple objective models that arise quite naturally from the classic theory of calculusv of variations. We then present an application of this theory to financial portfolio management.

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# A problem of reconstruction of discontinuities of a function given in attenuated medium by integrals along geodesics

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A problem of reconstruction of discontinuities of a discontinuous function by its known attenuated ray transform. A mathematical model of tomography including a refraction and internal sources, which assumed to be known, is considered. The main task of the formulated problem is to reconstruct a distribution of internal sources $f$ by its ray integrals. Our more narrow goal consists in visualization of a set of discontinuities of function $f$. One of approaches here is a visual representation of set of the points at which the values of certain operator, called an indicator of discontinuities, becomes infinite.

The indicators of discontinuities was constructed and applied successfully earlier [1] for recovery of discontinuities of scalar, vector and 2-tensor fields, but a synchronous influence of refraction and absorption to the reconstruction of discontinuities was not investigated. The model of "refractive tomography with internal sources" is investigated now by tools of mathematical modeling. Our first step consists in a calculation of the attenuated ray transform along geodesics. The results are used as the data at application to them newly constructed indicators of discontinuities in order to establish an influence of refraction and absorption to visualization of function discontinuities.

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# SS-ASQE Analogue Signals In Quantum Environments: The Physics and Mathematics of Propagation and Control

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# A nonlinear-master-equation model for quantum metamaterials

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The concept of a quantum metamaterial (QMM) was introduced in [1] (see also [4]) and subsequently realized in experiment [5]. In brief, a QMM is an engineered quantum structure, typically an array of qubits, whose particular physical characteristic, e.g. the optical refraction index, depends on its quantum state. When the quantum state of a QMM is changed, the physical characteristic in question will change significantly. The state of a QMM may be controlled via an external circuit, but it will also be affected during interaction with the ambient electromagnetic field or the passing signal. Here, we consider a master equation approach to developing quantitative models of such interactions and analysing the interactive dynamics.

Suppose a wave packet comes in contact with a QMM. During interaction its state entangles with the state of the QMM which in turns alters the QMM's properties. We describe such a process within the framework of a master equation. Namely, let the effect of the QMM on the environment be characterized by a collection of Lindblad operators, say, $L_j$, $j = 1,2,\ldots J$, which depend on the state of the QMM in some implicit manner. Let the wave packet (field subsystem) be characterised by the evolving mixed state $\rho = \rho(t)$. Its dynamic is captured by a *nonlinear* master equation, namely:

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H,\rho] + \sum_j \{L_j \rho L_j^\dagger - \frac{1}{2}L_j^\dagger L_j \rho - \frac{1}{2}\rho L_j^\dagger L_j\} \quad \text{wherein: } L_j = L_j(\rho). \tag{1}$$

The fundamental question is what constitutes a proper selection of the operator maps $\rho \mapsto L_j(\rho)$. In other words, how should the Lindblad operators depend on the state variable of the quantum subsystem representing the wave packet (alternatively, in the Heisenberg picture, on an observable pertaining to the subsystem)? One approach to this problem would be via first-principles based modelling of the QMM and the encompassing composite system. However, here we choose to address the problem from a more general standpoint of mathematical amenability. Namely, we examine the question of well-posedness of the initial value problem (1) with $\rho(0) = \rho_0$ for particular choices of the "feedback loop" maps $\rho \mapsto L_j(\rho)$.

Our numerical simulations and analyses rely crucially on the concept of the Q-transform [3]. On the one hand, the Q-transform is used to define amenable feedback loop maps. On the other hand, it is a fundamental tool of analysis as it furnishes the appropriate notion of regularity and allows formulation of well-posedness hypotheses for flows of type (1). To our knowledge, such evolution equations are conceptually novel, although they display some similarity with other operator evolution equations, see e.g. [2] and references therein.

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# Examples of quantum-dynamical nonlaws and their properties

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Nonlinear operator equations admit a number of applications in the area of quantum system modelling and are gaining in importance in view of the recent discovery of quantum metamaterials, [1], [2], [3]. The purpose of this work is to examine the mathematical nature of such equations, possibly going outside the canonical quantum theory or natural quantum system dynamics. Our focus is on Heisenberg type equations for the evolution of a quantum observable (or state), say $F$, that include a nonlinear term, e.g.

$$\frac{d}{dt}F = \frac{i}{\hbar}[\mathscr{H}, F] + F - F^2, \tag{1}$$

where $\mathscr{H}$ is a $N$-qubit Hamiltonian. For the purpose of this work we call (1) the Quantum Logistic Operator Equation (QLOE). We analyse the QLOE using an approach similar to that developed in [4] and find an explicit recursive formula for the solutions. Also, we apply the Q-transform approach, see [5], to carry out a type of harmonic analysis of the observables and to visualize the main features of their dynamics. While (1) is an example of a quantum *nonlaw*, i.e. an "accidental" generalization (cf. [6]), we consider its analysis as training for a general approach encompassing physical cases.

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# Expansion in large coordination number for quantum lattice systems

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The quantum lattice systems are encountered in many field of physics: solid states, ultra-cold gas and quantum meta-materials. The typical examples are the Bose or Fermi Hubbard models, or the Heisenberg spin model. An important application of these models is towards the investigation of essentially non-equilibrium and non-stationary effects such as quenching in a cold gas or evolution of a quantum annealer.

Our investigation is based on the general approach of 1/Z expansion (where Z is the lattice coordination number [1-4]). This formalism provides a general framework for building a hierachy of equations for the reduced n-site density matrices, which allows a systematic approach to the calculation of the equilibrium properties [3, 4] as well as to describe its non equilibrium dynamics [1, 2]. In our latest work [4], we use the 1/Z expansion to determine the ground state and the quench dynamics of the quantum Ising model in one, two and three dimensions. Our method reproduces quite well the physics of this model such as the quantum phase transition between the paramagnetic and ferromagnetic phases or also the excitation spectrum. Such a model describes the dynamics of an array of quantum magnetic moments (e.g., qubits) perturbed by an external magnetic field under the conditions of long de-coherence time. Such structures containing over 2000 qubits are being currently produced for the use as quantum annealers, but despite intensive research the question of the degree of their "quantumness" and the character of their evolution remains open [5]. Our recent results [4] provide insight into the non-equilibrium correlations in these devices.

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# Image denoising via Redundant Quantum Channels

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It was demonstrated in [1] that a natural image can be denoised via a quantum evolution schema. Our main purpose here is to test whether any advantage can be found in utilizing a redundant processing schema, wherein the quantum process is carried out in a variety of nonequivalent ways and subsequently post processed and averaged. To this end, we utilize the phenomenon of broadband redundancy, reported in [2]. As shown in Eqs. (1, 2), first, the classical information — consisting of a clear image $x_o$ with an addition of white noise $n_k$ (independent samples for $k = 1,\dots N$) — is encoded in select different ways into $N$ quantum observables. Second, these observables are evolved via the Lindblad master equation (LME) in parallel in $N$ identical quantum channels. Finally, the observables are back-converted into images (called $y_k$), subsequently post processed via nonlinear optimization (yielding $x_k$), and averaged, yielding the final recovered value $x_{rec}$.

$$L_k = Q^{-1}_{\sigma+it_k} D_T Q_{\sigma+it_k} \qquad y_k = L_k(x_o + n_k) \tag{1}$$

$$x_k = \arg\min_x \left( \frac{1}{2}\|L_k x - y_k\|^2_{l_2} + \alpha \|TV(x)\|_{l_1} \right) \qquad x_{rec} = \frac{1}{N}\sum_{k=1}^{N} x_k \tag{2}$$

Here $L_k$ is the $k^{th}$ measurement matrix, $Q_{\sigma+it_k}$ and $Q^{-1}_{\sigma+it_k}$ are used to represent an image as a quantum observable and vice versa, $D_T$ is the LME's transition matrix from time 0 to time $T$, $TV$ is the total-variation operator defined in [3], and parameter $\alpha$ is used to balance the data fidelity and regularization terms. A typical result is shown in Fig. 1.

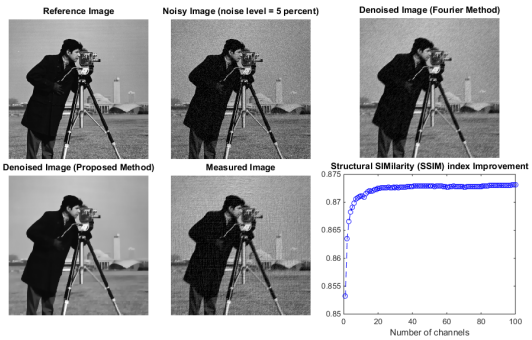


Figure 1: Visual and structural performance evaluation of the proposed algorithm

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# Mean Field Adiabatic Quantum Computation

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The general goal of a quantum computers is to solve a discrete optimization problem which is a search for the ground state of a spin-glass like classical Ising model where the spin-spin couplings are not identical[1, 2]. This optimization is very common in mathematics, economics and engineering. When N denotes the total number of sites, the number of choices, $2^N$, leads to an exponentially long solution time and nonlinear optimization problem. Quantum annealing is a procedure that reaches the ground state of a classical Ising model by turning off adiabatically the transverse magnetic field. This alternative quantum computation method solves the optimization problem for the classical Ising model faster if implemented on a quantum device.

In this paper we address the issue of the specific role played by the quantum correlations by analyzing the consequences of their suppression using the mean field description. The latest corresponds to the leading order in the large coordination number expansion characterizing the general lattice Hamiltonian. It assumes that the coordination number Z (number of couplings of a given site with other sites) is large, so that next order corrective terms $1/Z^l$ give decreasingly smaller contributions to the lattice system dynamics.

This expansion provides a general framework of hierarchical equations for n-sites reduced density matrices allowing us to determine systematically equilibrium properties such as the ground state [3, 4] as well as nonequilibrium dynamics [5, 6]. It has resulted in an efficient controllable approximation scheme for determining the ground state and the quench dynamics of a uniform quantum Ising model for any dimension, including the quantum phase transition between the paramagnetic and ferromagnetic phases and the excitation energy spectrum [3].

The obtained results from this "mean field" adiabatic computation are compared and discussed with those of the non-linear discrete optimization method and provide useful insights to the influence of correlations in the efficiency of quantum computation.

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# The fractional Fourier processing of signals associated with quantum information analysis

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Fractional Fourier processing methods, including fractional Fourier transform (FRFT) and the linear canonical transform (LCT), have been paid much more attentions in quantum information [1] community and many other research fields. The FRFT and LCT are fractional of the standard Fourier transforms (FTs) [2], which are much more flexible in terms of the parameter degree than that of FT. The LCT for a signal $s(t)$ is defined as following [3]

$$S_A(u) = \mathscr{L}_s^A(u) = \begin{cases} \int_{-\infty}^{+\infty} s(t) K_A(u,t), & b \neq 0 \\ \sqrt{d} e^{j(cd/2)u^2} s(du), & b = 0 \end{cases} \tag{1}$$

where

$$K_A(u,t) = \frac{1}{\sqrt{j2\pi b}} e^{j(\frac{du^2}{2b} - \frac{ut}{b} + \frac{at^2}{2b})} \tag{2}$$

with parameter matrix $A = (a,b;c,d)$ and parameters $a,b,c,d$ are real numbers satisfying $ad-bc=1$, i.e. $det(A) = 1$. When $A = (\cos\alpha, \sin\alpha; -\sin\alpha, \cos\alpha)$, LCT reduces to FRFT, and it will yields to the traditional FT when $A = (0,1;-1,0)$. Dirichlet matrix operators (D-operators for short) is another important tool in the fields of signal analysis and quantum processing. It has been demonstrates that such operators have an exceptional structure which enables efficient numerical implementation via a lifting schema at the cost of $O(N \log N)$. These are the only fast transforms other than the Fourier or the wavelet transforms known to-date [4]. How to use the advantage of D-operator and fractional transform techniques to deal with the non-stationary signal and apply them for quantum information processing, is one of interesting and important topics in modern information processing community.

The aim of this paper is to investigate the relationship between the fractional transform techniques and D-operators, and then provide an overview of developments and research trends pertaining to the FRFT and LCT in quantum information processing. First, the paper introduces the definitions and properties of FRFT and LCT by operator approach [5], and D-operators are introduced as well. Second, the fractional D-operators are investigated based on the the physical interpretations of FRFT and LCT, and then the FRFT and LCT operators may be factorized by Dirichlet multiplication to improve the efficiency of digitization algorithm. Third, the potential applications of fractional Fourier processing in the field of signal processing and quantum information are discussed in details. It should be noted that the fractional Fourier processing methods can be more efficient by introducing the fractional D-operators. Its practical applications in quantum information are expected to grow significantly in years to come, given that the FRFT and LCT offers many advantages over the traditional Fourier analysis.

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M.A. Qureshi, J. Zhong, P. Mason, J.J. Betouras, A.M. Zagoskin

Pechukas-Yukawa formalism for the description of quantum coherent structures.

Abstract:

Quantum technologies 2.0 are based on large quantum coherent systems out of equilibrium. Description, simulation and characterization of such systems is intrinsically difficult. In the Pechukas-Yukawa formalism for externally perturbed quantum systems the energy levels dynamics is mapped on that of a fictitious classical one-dimensional gas, which is described by a generalized Calogero-Sutherland system of equations. Here we extend the formalism to the case of an arbitrary nonstationary evolution by developing the BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) chain of equations for the hierarchy of distribution functions for the "gas" supplemented by the equations for the level occupation numbers and transition amplitudes. We show that the formalism can form the basis for a perturbation scheme, which takes into account remote quantum correlations in the underlying physical structure.

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# Quantum transport in a superlattice driven by a high-frequency acoustic wave.

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A quantum particle transport induced in a spatially-periodic potential by a propagating plane wave has a number important implications in various quantum systems such as semiconductor superlattices [1] and cold atoms in optical crystal [2]. Our work is dedicated to the effects of hypersonic acoustic strain wave on the quantum charge transport in a semiconductor superlattice. While travelling along the axis of the SL, the acoustic wavepacket affects the electron tunnelling, and thus determines the electric current through the device. In our theoretical calculations, we applied a kinetic description of the directed transport in a superlattice, and utilize the exact path-integral solutions of the semiclassical transport equation. This approach allowed to reveal the regimes and the instabilities governing the miniband electron transport induced in a periodic superlattice potential by a propagating acoustic wave. Our results suggest that a GHz (hypersonic) acoustic wave can create fast electron dynamics in the superlattice, thus generating sub-millimeter electromagnetic waves, even when no static electric field is applied. These findings were supported by direct quantum simulations, which also demonstrated a good agreement with experimental measurements of the current-voltage characteristics and the current pulse shape in superlattices under action of a high-frequency strain pulse train.

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# Quantum Zeno dynamics of qubits in a squeezed reservoir: effect of measurement selectivity

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A complete suppression of the exponential decay in a qubit (interacting with a squeezed vacuum reservoir) can be achieved by frequent measurements of adequately chosen observables. The observables and initial states (Zeno subspace) for which the effect occurs depend on the squeezing parameters of the bath. We show this effect to be substantially different for selective and non-selective measurements. In either case, the *approach* to the Zeno limit for a finite number of measurements is also studied numerically. The calculation is extended from one to two qubits, where we see both Zeno and anti-Zeno effects depending on the initial state. The reason for the striking differences with the situation in closed systems is discussed.

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# Time dependent real-space Renormalisation Group Treatment of the Random Transverse-Field Ising Model

P. Mason, A. Zagoskin, J. Betouras

*Loughborough University, UK*

A quantum adiabatic computation is one in which the governing Hamiltonian is slowly varied in time, starting from an initial Hamiltonian for which the ground state is known, and ending with a final Hamiltonian, the ground state of which encodes our desired solution. Throughout the evolution we always remain in the ground state. Such a technique to establish the solution of a computational task in a quantum simulation, together with quantum annealing, can be extremely effective, and is employed for instance in the D-wave devices.
Here we consider a renormalisation group treatment [1, 2] on the strongly disordered random one-dimensional transverse-field Ising spin chain where the bonds $J_{ij}$ and horizontal fields $h_i$ are time-dependent and chosen to reflect an adiabatic evolution of the governing Hamiltonian. Under the condition that the renormalisation process occurs at fixed time, a set of coupled second order, nonlinear PDE's can be written down in terms of the random distributions of the bonds and fields. Solution of these flow equations at the relevant critical fixed points leads us to the establish the critical behaviour of the flow as the Hamiltonian is adiabatically evolved. We will present these critical flows as well as discussing the issue of duality, before making connections to quantum adiabatic computations.

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# SS-CC Computational Chemistry

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# Effect of charges on the stability of non-covalent complexes: A computational study of a DNA duplex stability in charged nanodrops

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Nanodrops with excess charge play a critical role in aerosols and electrospray ionization (ESI) processes. We analyze the desolvation mechanism of a double-stranded deoxyribonucleic acid (dsDNA) from an aqueous nanodrop studied by using atomistic molecular dynamics methods (Fig. 1). We examine the increase in ion concentration and the distinct droplet morphologies arising from the charge-induced instability and explore in detail an extensive set of nanodrops with excess negative charge each comprises a dsDNA, Na and Cl ions at various concentrations (Refs. [1]). We find that for the square of the charge to volume ratio above that of the Rayleigh limit the droplet attains distinct spiky morphologies that disperse the charge in larger volume than that of the spherical drop (Refs. [2]). In the presence of $Na^+$ and $Cl^-$ ions, Na cations form adducts with the double helical DNA in the minor groove, which helps preserve the duplex state in the gas phase. In a droplet with a net charge that is less negative than 50% of the dsDNA charge, the DNA maintains a double-stranded state in the gas phase. Several of our findings are in good agreement with experiments, though the spiky droplet morphology due to the charge-induced instability invites for new experiments. The results illustrate the association properties of complexes of macromolecules in droplet environment, which are critical intermediates in electrospray ionization experiments.

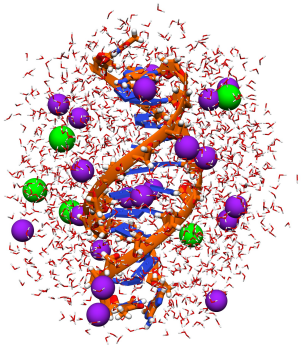

Figure 1: A model representation of a typical nanodrop with excess negative charge. The nanodrop comprises a $[dsDNA]^-$20 $Na^+$ ions (purple spheres), and $Cl^-$ ions (green spheres) in TIP3P water models.

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# Interactions of Simple Ions in Atmospheric Aerosols

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Atmospheric aerosols are a growing topic of interest due to their relevance to climate and pollution, and consequently health, air quality, and visibility. Many aerosol particles contain inorganic compounds in the form of electrolytes, with the largest contribution occuring from salt in sea spray aerosols (Ref [1]). The interactions of these ions in and with aerosols are often difficult to study experimentally due to the variety of sizes, charges, constituents and short life-times of the clusters. Computer simulations offer a better look into the reactions that take place in charged aerosol droplets. In particular, the small size of the droplets (sub-3nm to micrometer diameters) can be accurately depicted with molecular level modelling and simulations can capture rapid changes including fragmentation mechanisms and evaporation of such charged systems (Ref [2]). Ion interactions in aerosols are of interest because the highly fluctuating environment of small droplets may permit reactions of a different nature than those occuring in bulk solution. Reasearch done here, aims to illuminate reaction pathways of simple ions within the aqueous environment of an atmospheric aerosol through molecular dynamics simulations.

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# Stability of a Transient Protein Complex in a Charged Aqueous Droplet with Variable pH

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Electrospray ionization mass spectrometry (ESI-MS) has the potential to become a high-throughput robust experimental method for the detection of protein-protein equilibrium constants[1-2]. Poorly understood processes that affect the stability of weak non-covalent protein complexes in the intervening droplet environment is a significant factor that precludes the advancement of the method. We use atomistic molecular dynamics simulations to study the stability of a weak transient complex of ubiquitin and ubiquitin-associated domain (RCSB PDB code 2MRO[3]) in an aqueous droplet with changing size and charge concentration. We present evidence that a weak protein complex changes conformation and may dissociate in shrinking droplets even before desolvation[4]. Then the droplets containing these dissociated proteins divide. Our findings suggest that in some cases ESI-MS does not measure the correct association constants. The study intends to stimulate research for systematic development of experimental protocols that stabilize weakly bound protein interfaces in droplets.

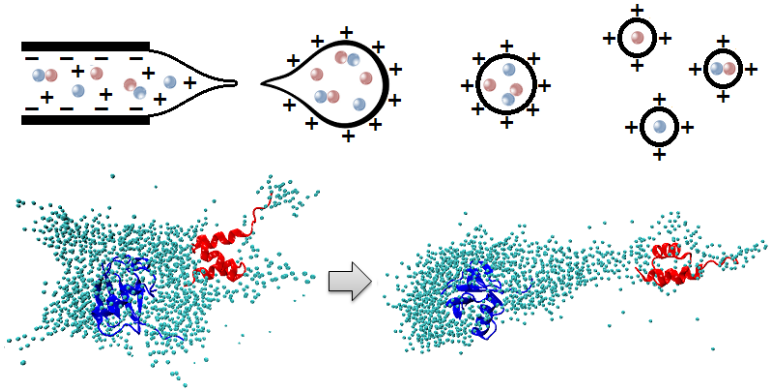

Figure 1: Protein complex dissociation during the process of electrospray ionization. The ubiquitin molecule is colored in red, the ubiquitin-associated domain in blue, and the oxygen sites of water molecules (small spheres) in light blue.

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# Studying properties of RNA nanotubes with atomistic-to-continuum models

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RNA self-assembled structures have many important applications in biomedicine. In order to understand their features in such applications, it is necessary to have thorough understanding of the properties of RNA nanoclusters obtained from self-assembly of their building blocks. Earlier, using all atom molecular dynamics simulations, the modeling of RNA nanotubes up to the size of 20nm has been carried out and their properties have been analyzed [1, 2]. Recently, the RNA nanoscafolds have been modeled via self-assembly of RNA building blocks to study their stability and potential application in biomedicine [3]. The properties so far studied are for small scale applications. In order to study the properties at larger scales we have developed continuum models of the RNA nanotubes based on atomisitic information. In the present work we demonstrate how to calculate elastic properties of RNA nanotubes using finite element method based on these newly developed models. Specifically, we take a typical RNA nanotube of size 80 nm that has been obtained from the self-assembly of 20 RNA nanorings. We have analyzed in detail strain tensor components as functions of temperature, as well as the displacement distributions (e.g. Fig. 1). From the results it is clear that the $\varepsilon_{11}$ component of the strain tensor is decreasing as the temperature increases, whereas other components, $\varepsilon_{22}$ and $\varepsilon_{33}$, are found to increase with temperature. This indicates a compression of the RNA nanotube along one principal axis and the elongation along two other principal axes. The distributions of displacement and the variations of strain tensors provide further insight into the stability of RNA nanotubes.

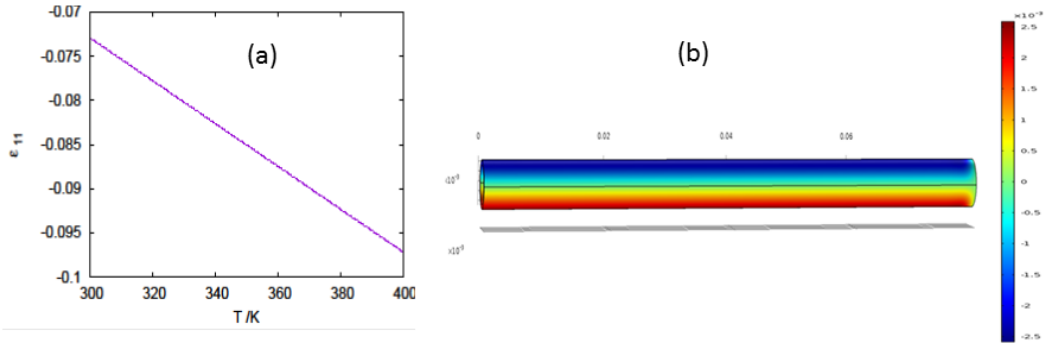


Figure 1: (a) Variation of the strain tensor component, $\varepsilon_{11}$ of RNA nanotube as a function of the temperature. (b) The displacement distribution along the entire volume of the RNA nanotube.

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# SS-CDAHS Complex Data Analysis in Health Science

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# A New Constrained Mixture Models for Drug Discovery Data

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It has been well-known that Statistics has played a very important role in drug discovery: facilitate and speed up the drug finding process. Statistical learning in drug discovery seeks a good classifier that separates chemical compounds into active and inactive classes. The active compounds are those that inhibit disease virus and are taken as drug candidates. However, the characteristics of drug data imply many challenges for structure modeling and identification of active compounds. Among these characteristics are the rarity of active compounds, the large volume of compounds tested by high-throughput screening, sub-set governed activity and the complexity of molecular structure and its relationship to activity. Due to the challenges of drug discovery data, we develop a new statistical learning model based on mixture models: Constrained Mixture Discriminant Analysis (CMDA) model. This method is designed to catch multiple mechanisms that lead to activity, explore the subsets of descriptors and be easily interpreted (e.g. identify important descriptors). The Expectation-Maximization is used to estimate the parameters of the CMDA model. Comparing to the popular MclusteDA model, CMDA outperforms MclustDA in terms of the parameter estimation and the active compound identification.

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**Title**

Comparing Clostridium difficile infected patients before and after a treatment using loops in DNA sequences

**Abstract**

To analyze data that are presented as measure of similarity or dissimilarity, one of appropriate statistical methods might be cluster and classification analysis. Computational topologists recently developed a method, called persistent homology. Persistent homology studies the evolution of topological features in a space as a parameter increases. Persistent homology captures higher order features beyond clustering. There are three descriptive statistics of persistent homology, namely barcode, persistence diagram and persistence landscape. Persistence landscape is useful for statistical inference as it belongs to a space of p-integrable functions, which is a separable Banach space (Bubenik 2015). We apply tools in both statistics and computational topology to DNA sequences taken from clostridium difficile infected patients and their donors. Our statistical and topological data analysis is able to detect interesting patterns among patients and donors. It also provides visualization of DNA sequences in the forms of clusters and loops. This research is collaborated with Pavel Petrov, Stephen Rush, Zhichun Zhai, Christine Lee, and Peter Kim.

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# Data Mining for Patterns of User Engagement with a Mobile App (Manage My Pain) for Monitoring and Tracking Chronic Pain

Quazi Abidur Rahman[1], Meysam Pirbaglou[2], Tahir Janmohamed[3], Paul Ritvo[2,5], Jane M. Heffernan[1], Hance Clarke[4], Joel Katz[2,4,5]

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Pain is one of the most prevalent health-related concerns and is among the top three most common reasons for seeking medical help. Scientific publications describing analysis of data collected from pain tracking and monitoring apps are important to help consumers and health care professionals select the right app for their use. The main objectives of this study are to (1) discover user engagement patterns of a commercially-available app, Manage My Pain, using clustering methods and (2) identify the association between several attributes characterizing individual users and their levels of engagement. User engagement was defined by two key features of the app - longevity (number of days between the first and last pain record) and number of records. Users were divided into 5 user engagement clusters employing the *k-means* clustering algorithm (Fig. 1). Each cluster of users was characterized by six attributes: gender, age, number of pain conditions, number of medications, pain severity, and opioid use. Z-tests and chi-squared tests were used for analyzing categorical attributes. Effects of gender and cluster on numerical attributes were analyzed using 2-way ANOVAs and were followed up by pairwise comparisons using Tukey HSD. The results from this study show that although most users of the app reported being female, male users are more likely to be highly engaged in the app. In addition, users in the most engaged clusters self-reported: a higher number of pain conditions; a higher number of current medications; and a higher incidence of opioid usage. The present results may also reflect the fact that the highly-engaged males are older than highly-engaged females. The high engagement by males does not appear to be driven by pain severity which may, in part, be the case for females. Based on these results, we suggest that use of a mobile pain app may be relatively more attractive to highly-engaged males than highly-engaged females, and to those with relatively more complex chronic pain situations.

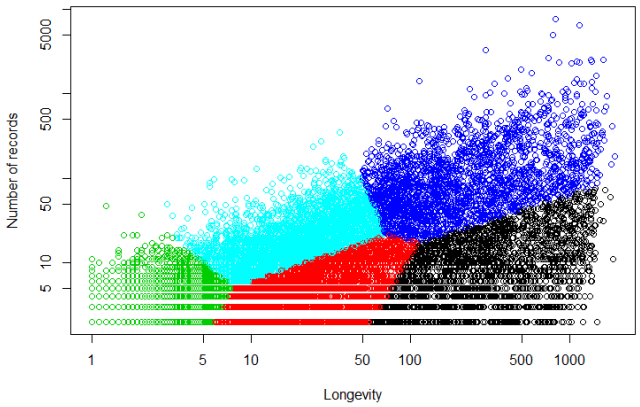


Figure 1: Clustering solution using 5 clusters (Blue: high longevity, high number of records; Black: high longevity, low number of records; Cyan: low longevity, high number of records; and Red and Green: low longevity, low number of records)

## Developing two deterministic and robust models for the home health care routing and scheduling problem


## Abstract

This paper presents an integrated formulation and a solution method for the daily staff routing and service scheduling developed for home health care companies. The proposed model is *mixed integer linear programming model* (MILP), in which many real situations are considered to make the model more practical than existing routing and scheduling models. For example, different qualifications, diverse vehicles, different requirements for patients, possible temporal interdependencies between services, time windows for both patients and staff members, and *continuity of care* (*CoC*) are taken into account. We also added some essential constraints related to blood sampling requirements. In this model, the total real and virtual costs are minimized in the objective function. Furthermore, we have proposed a *genetic algorithm* (GA) to find near-optimal solutions for the mathematical model in a reasonable time. The numerical results demonstrate that the runtimes of GA applied on different sets of randomly generated test instances are significantly less than those obtained through exact method for medium and large sized problems. As a result, the scheduling and routing policies obtained by the solution scheme can be more proper for the studied problem.

The emphasis of significant alterations in providing home health care services has incited more attention in designing robust logistics networks. This paper proposes a robust optimization model for handling the uncertainty in transportation times and duration times for a routing and scheduling problem in home health care. First, a deterministic mixed integer linear programming model is developed for designing a logistics network. Then, the robust counterpart of the proposed model is presented through the robust optimization theory. Finally, to evaluate the robustness of the solutions obtained, they are compared to those generated by the deterministic model in a number of test instances with different sizes.



**Key-Words:** Home health care, Routing and scheduling, Double services, Temporal interdependencies, robust optimization, Genetic algorithm.

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# Inferring Direct Genetic Effects in Directed Acyclic Graphs Using Estimating Equations

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Many genetic associations have been identified with disease phenotypes through genetic association studies. However, the associations do not infer the causal genetic effects. It is necessary to consider all potential effects between the genetic variants, phenotypes, and confounding factors in order to make valid statistical inference on genetic effects. In this study, under a directed acyclic graph (DAG) setting (see Refs [1,2]), we propose a new method using estimating equations to make inference on the direct genetic effect on the primary phenotype. The proposed causal inference method based on estimating equations (CIEE) using robust sandwich standard errors (see Ref [3]) removes the effect of intermediate phenotypes from the primary phenotype and adjusts the model for measured and unmeasured confounders. We consider settings where the continuous primary phenotype is completely observed and is subject to censoring. We evaluate CIEE and compare it with traditional methods based on multiple regression models (see Refs [1,2]), the structural equation modeling method (see Ref [4]), and the G-estimation method (see Refs [1,2]) through a simulation study for the analysis of continuous and time-to-event traits as primary phenotypes. Simulation studies show that CIEE successfully removes the effect of intermediate phenotypes, gives consistent genetic effect estimates, and is robust against unmeasured confounding of the indirect effect through observed factors. The proposed Wald-type test statistic obtained through CIEE to test the absence of genetic effect has valid type I error. CIEE provides valid inference even if the distribution of the primary phenotype is misspecified. Other methods may fail under some scenarios. The traditional methods based on multiple regression models give biased genetic effect estimates when there is unmeasured confounding. The structural equation modelling method might yield biased genetic effect estimates when the amount of unmeasured confounding is moderate or substantial or when the DAG is misspecified. The G-estimation method proposed for analyzing time-to-event primary phenotypes (see Ref [1]) does not remove the effect of the intermediate phenotypes and gives biased direct effect estimates. In the analysis of the Genetic Analysis Workshop 19 dataset (see Ref [5]), we estimate and test genetic effects on blood pressure accounting for intermediate gene expression phenotypes. The results show that CIEE can identify genetic variants that would be missed by traditional regression analyses.

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# Regression-based mixture models for microbiome data

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The human gut microbiome is a source of great genetic and metabolic diversity. Microbiome samples which share similar biota compositions are known as enterotypes. Exploring the relationship between biological/ environmental covariates and the taxonomic composition of the gut microbial community can shed light on the enterotype structure. Dirichlet-multinomial models have been previously suggested to investigate this relationship, however these models did not account for any latent group structure. Here, a finite mixture of Dirichlet-multinomial regression models is proposed and illustrated. These models allow for accounting for the enterotype structure and allow for a probabilistic investigation of the relationship between bacterial abundance and biological/environmental covariates within each inferred enterotype. Furthermore, a generalization of these models is also proposed that can incorporate the concomitant effect of the covariates on the resulting mixing proportions.

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# Resampling Techniques for Estimation and Inferences for Variances

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With the presence of a complex sampling design, which may be informative, inference on the population variance can be challenging. In this paper, we extend a resampling technique called artificial population bootstrapping (APB) put forward by Thompson and Wang (Ref [1]) to investigate inference on the finite population variance.

Inferential issues that include the point and interval estimation of a population variance will be resolved using the APB technique. We propose regression techniques to lower the biases of estimators of the variance of the analogue of sample variance under complex sampling designs. Such regression techniques take advantage of the structures of the artificial populations and its resamples in an APB procedure and provide very elegant results in terms of bias correction when estimating a variance. Simulation studies have been carried out to examine the quality of the methodology.

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# Statistical Inferences on Average Precision and ROC Curves

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There are two kinds of medical tests: screening tests and diagnostic tests. The purpose of a screening test is to determine whether an asymptomatic individual has a certain disease or not, while diagnostic tests are used to confirm the disease status.

To evaluate the effectiveness of a diagnostic test, the gold standard is the receiver operating characteristic (ROC) curve which traces the tradeoff between sensitivity (true positive rate) and specificity (true negative rate) as the decision threshold varies. When comparing performance of medical tests, a single numeric performance metric, the Area Under the ROC Curve (AUC), is the most widely used performance measure. As a summary measure, AUC is independent of the prevalence of the disease.

When evaluating screening tests, clinicians adopt the AUC ignoring the fact that the prevalence is generally low for many screened diseases in asymptomatic populations. The purposes of screening tests are to identify diseases in their early stages, when no symptoms are present, so as to facilitate early intervention with the hope to improve outcomes. Therefore, a performance metric that accentuates the true positive rate at the early part of the ROC curve is more attractive than a metric that treats the true positive rate equally important across the entire curve such as the AUC. For the same type of evaluations, a different metric known as the average precision (AP) is used much more widely in the information retrieval (IR) community, where the task is to retrieve relevant documents from a collection of documents.

The AUC is the area under the ROC curve, and the AP is the area under the so-called Recall-Precision curve. Like the AUC, the AP is a single numeric performance metric that does not require us to commit to a decision threshold prior to the analysis. Little has been done on making statistical inferences on the AP. To fill the gap, we study both metrics in some depths in order to elucidate their difference and relationship. More specifically, we explain mathematically why the AP may be more appropriate if the earlier part of the ROC curve is of interest and hence is more appropriate for screening tests (see [1]). We also proposed a framework to make statistical inferences on the AUC and the AP based on the multinomial model and the delta method. The performance of this framework is demonstrated with real-world examples concerning the evaluation of protein biomarkers for prostate cancer and the assessment of digital versus film mammography for breast cancer screening (see [2]).

For ROC curve fitting and inference, we propose two new methods based on the ranks of the two classes for estimating the bi-normal parameters in ROC analysis: the method of quantiles and the maximum likelihood method based on quantiles. Using both simulation and real-world examples, we study the performance of the two proposed quantile methods and illustrate the use of the quantile methods in evaluating medical tests.

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# SS-CNT Computational Number Theory

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# Complexity of Arithmetic with Multi-Dimensional Digit Representations

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Digit representations for vectors can be defined using a similar algebraic structure as digit (positional) representations for integers and real numbers. We consider as our base (radix) a square matrix $A \in M_n(\mathbb{Z})$ whose eigenvalues each satisfy $|\lambda| > 1$, called a *dilation matrix*. A set $D$ of coset representatives of $\mathbb{Z}^n/A(\mathbb{Z}^n)$ may be chosen as digits. We then consider vectors with integer entries represented by finite sums $\mathbf{k} = \sum_{i=0}^{m} A^i d_i, d_i \in D$ [3]. As with one-dimensional digit representations, the standard multi-digit addition and subtraction algorithms can be used to add or subtract multi-digit vectors in this representation, referring to an appropriate addition table for single-digit additions. However, as shown in the thesis of M. ALmutairi [2], addition of $m$-digit vectors may be $O(m^2)$ rather than $O(m)$ as is the case for standard one-dimensional multi-digit addition. The primary cause of this extra complexity is that the digit sets for multi-dimensional radix representations that are useful in other applications are centered around $\mathbf{0} \in \mathbb{Z}^n$, so single-digit addition involves subtraction as well as addition. We show that for certain classes of digit sets, the complexity of multi-digit addition will always be $O(m^2)$, but no worse. We also show that this can be remedied in part using a base-complement algorithm, generalizing the two's complement algorithm for subtraction of multi-digit binary numbers.

Multi-dimensional radix representations were originally formulated to study properties of multi-dimensional wavelets [3]. They can be used to define iterated function systems whose attractors tile $\mathbb{R}^n$ under translation by $\mathbb{Z}^n$ or a sub-lattice. They are thus closely tied to the study of more general number systems and digit representations from the area of ergodic number theory [1, 4]. In addition to the interdisciplinary applications of multi-dimensional radix representations in these other areas of mathematics, the development of positional number systems for the natural numbers was a major development in the history of mathematics, enabling effective algorithmic computation both by hand and using modern computers. A reasonable question, then, is if multi-dimensional radix representations enable any new computational advances over current algorithms for vector arithmetic. The complexity of converting between traditional component-wise vector representations and multi-dimensional radix representations is an initial hurdle that makes arithmetic with multi-dimensional radix representations not computationally useful for small calculations with data supplied in traditional vector notation. However, multi-dimensional radix representation still has the potential to be useful when many calculations will be performed on vectors of high dimension, or when data can be initially collected or supplied in multi-dimensional radix representation without requiring a conversion step. Although results obtained to date have been of a more fundamental or preliminary nature, this talk will also review the current status of ongoing work investigating this motivating question of whether multi-variable radix representations can be useful in computational applications.

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# Computing Elliptic Curves Over $\mathbb{Q}$

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In the 1950's and 1960's, Taniyama and Weil asked whether all elliptic curves over $\mathbb{Q}$ of a given conductor $N$ are related to modular functions. While this conjecture is now known as the Modularity Theorem, until its proof in 2001, attempts to verify it sparked a large effort to tabulate all elliptic curves over $\mathbb{Q}$ of given conductor $N$.

Let $K$ be a number field and let $S$ be a finite set of primes of $K$. In 1963 Shafarevich proved that there are at most finitely many $K$-isomorphism classes of elliptic curves defined over $K$ having good reduction outside $S$. In 1970, Coates [2] proved an effective version of this result when $K = \mathbb{Q}$ using linear forms in $p$-adic and complex logarithms. Many of the early attempts to compute elliptic curves over $\mathbb{Q}$ have much in common with the arguments of [2], in that they reduce the problem to solving a number of *Thue-Mahler equations*. These are Diophantine equations of the form

$$F(x,y) = u, \tag{1}$$

where $F$ is a given binary form of degree at least 3 and $u$ is an *S-unit*, that is, an integer whose prime factors all lie in $S$.

There are very few, if any, subsequent attempts in the literature to find elliptic curves of given conductor via Thue-Mahler equations. Instead, many of the approaches involve a completely different method to the problem, using modular forms. Currently, using this approach, all elliptic curves over $\mathbb{Q}$ of conductor $N$ have been determined for $N \leq 390000$, the bulk of this work being attributed to Cremona (see e.g. [3]).

In this talk, we describe an algorithm to compute elliptic curves over $\mathbb{Q}$ using Thue-Mahler equations. In particular, let $S = \{p_1, \ldots, p_k\}$ be a set of rational primes necessarily containing the prime 2. Suppose that we wish to find models for $\mathbb{Q}$-isomorphism classes of elliptic curves over $\mathbb{Q}$ with given conductor $N = p_1^{\alpha_1} \cdots p_k^{\alpha_k}$, where the $\alpha_i$ are positive integers. In [1], Bennett and Rechnitzer show that this problem reduces to solving a number of Thue-Mahler equations. To compute all such equations, there exists a practical method of de Weger [4] using bounds for linear forms in $p$-adic logarithms and various reduction techniques. The goal of our approach is to compute elliptic curves up to some much larger bound than Cremona in the case K = Q, as well as to compute elliptic curves over K, where K is a number field, with bounded conductor. We describe our implementation of this method and discuss the key steps in used in our algorithm.

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# Computing zeta functions in average polynomial time

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Let $X$ be a smooth projective curve defined over a finite field of prime order $p$. Determining the number of rational points on $X$, or more generally, computing the zeta function of $X$, is a core problem in computational number theory with many applications. For curves of genus $g = 1$, Schoof [8] uses a CRT approach to obtain a polynomial-time algorithm; Schoof's algorithm has been generalized to curves of higher genus by Pila [7], with a running time that is polynomial in $\log p$ but exponential in $g$. Alternatively, $p$-adic approaches based on generalizations of Kedlaya's algorithm [6] yield a running time that is polynomial in $g$ but exponential in $\log p$. No algorithm with a running time that is polynomial in both $g$ and $\log p$ is currently known.

Now suppose $X$ is instead defined over the rational numbers, and consider the sequence of curves $X_p$ obtained by taking the reductions of $X$ modulo primes $p$ of good reduction up to some bound $N$. The problem of computing the zeta functions of all the $X_p$ naturally arises when one wishes to compute the $L$-function of $X$, or to study its Sato-Tate distribution. Harvey [1, 2] has shown that this problem can be solved in time quasi-linear in $N$; the average time to compute the zeta function of each of the curves $X_p$ is polynomial in both $g$ and $\log p$.

I will report on recent practical implementations of this algorithm [3, 4, 5], focusing in particular on curves of genus 3, both hyperelliptic and non-hyperelliptic, where we have obtained results that are dramatically faster than using either a CRT or $p$-adic approach to compute the zeta function of each $X_p$ individually.

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# Constructing hyperelliptic curves of genus 3 whose Jacobians have CM

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For cryptographic applications, it is convenient to, given a CM field, be able to construct an abelian variety with complex multiplication by an order in the ring of integers of that field.

It is currently well-understood how to do this in dimension 1, and a lot of progress has been done in dimension 2. We discuss here the challenges of constructing an abelian threefold with complex multiplication by the ring of integers of a sextic CM field and the work that has been done recently in this direction.

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# Counting elliptic curves with prescribed torsion over finite fields

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In this joint work with Nathan Kaplan, we present a geometric method that counts elliptic curves of a prescribed torsion, or a given Galois representation, over a given finite field.

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# Effective results on unlikely intersections of dynamical systems

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Unlikely intersections are a subject of much current interest in geometry. Masser and Zannier [2] proved the celebrated result that on the parametrized family of Legendre elliptic curves, two points with abscissae- 2 and 3 are simultaneously torsion for at most finitely many curves. This is an 'unlikley intersection,' as the set of parameters for which the two points are individually torsion is infinite but sparse. Like many problems in geometry, unlikely intersections have a natural analogue in dynamical systems. The simplest analogue of the Masser-Zannier problem is to replace the Legendre family with the parametrized family of quadratic polynomials $f_c(x) = x^2 + c$. As the dynamical analogue of torsion points is preperiodic points, Zannier asked at an AIM workshop in 2008:

> Are there infinitely many parameters $c$ such that $z = 0$ and 1 are both perperiodic under iteration of $f_c(x) = x^2 + c$?

Baker and DeMarco [1] answered this question in 2011, proving that this particular unlikely intersection is finite. However, their result was ineffective, as it gave no indication what parameters $c$ this set might contain.

The author recently introduced a metric of mutual energy for adelic measures associated to the Arakelov-Zhang pairing, using which one can provide an effective solution of this problem by obtaining a bound on the degree of the parameters $c$. Several computational issues arise in making these results effective, including computing a moduli of continuity for the Green's functions of the associated Mandelbrot sets. We will discuss the computational issues that arise in making such results effective.

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# Effective Sato–Tate under GRH

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Based on the Lagarias-Odlyzko effectivization of the Chebotarev density theorem, Kumar Murty gave an effective version of the Sato-Tate conjecture for an elliptic curve conditional on analytic continuation and Riemann hypothesis for the symmetric power L-functions. We use a stronger version of Chebotarev from the same Lagarias-Odlyzko paper to give a similar conditional effectivization of the generalized Sato-Tate conjecture for an arbitrary motive. As an application, we give a conditional upper bound of the form $O((\log N))^2$ for the smallest prime at which two given rational elliptic curves with conductor at most N have Frobenius traces of opposite sign. Then we will talk about the corresponding result for higher dimensional abelian varieties.

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# Efficient compression of SIDH public keys

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Supersingular isogeny Diffie-Hellman (SIDH) is an attractive candidate for post-quantum key exchange, in large part due to its relatively small public key sizes. Recent work of Azarderakhsh et al. [1] showed that SIDH public keys can be further compressed in size by around a factor of two, but with a significant performance penalty. We propose a range of new algorithms and techniques that accelerate SIDH public-key compression by more than an order of magnitude, making the compression process roughly as fast as a round of standalone SIDH key exchange, while further reducing the size of the compressed public keys by approximately 13%. These improvements enable the practical use of compression, achieving public keys of only 330 bytes for the concrete parameters used by Costello et al. [2] and further strengthening SIDH as a promising post-quantum primitive.

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# Elliptic Nets and Denominator Nets

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An elliptic net over $\mathbf{Q}$ is a function $w$ from $\mathbf{Z}^d$, satisfying

$$\begin{aligned} &w(p+q+s)w(p-q)w(r+s)w(r)+\\ &\quad w(q+r+s)w(q-r)w(p+s)w(p)+\\ &\quad\quad w(r+p+s)w(r-p)w(q+s)w(q)=0, \end{aligned}$$

for all $p,q,r,s \in \mathbf{Z}^d$. Stange proved that there is a close connection between elliptic nets over $\mathbf{Q}$ and elliptic curve $E/\mathbf{Q}$ with $d$ rational points $(P_1,\dots,P_d)$ on $E$. Intuitively, we think of $w(s)$ as the "denominator" of $s_1P_1+\cdots+s_dP_d$. However, one has to be careful when formalizing this intuition. In this talk, we define what we mean by denominator of a rational point of an elliptic curve, and we define a function we call *denominator net* using it. We then show how one can compute denominator net from elliptic nets and vice versa.

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# Explicit computations with the moduli space of abelian surfaces with a level 3 structure

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The Burkhardt quartic threefold is the projective hypersurface cut out by the equation

$$\mathscr{B}: y_0^4 + y_0(y_1^3 + y_2^3 + y_3^3 + y_4^3) + 3y_1y_2y_3y_4 = 0. \tag{1}$$

For a variety of reasons the geometry of the Burkhardt quartic has been studied for over a century. For example, $\mathscr{B}$ is birational to projective space, highly singular, and the unique quartic invariant of an action of $\mathrm{PSp}(4,3)$ on projective space. The number theoretic interest with $\mathscr{B}$ stems from the fact that most points on the Burkhardt quartic correspond to jacobians of genus 2 curves equipped with extra torsion structure. More precisely, an open subset of the Burkhardt quartic threefold is isomorphic to an open subset of the moduli space of principally polarized abelian surfaces with a full level 3 structure; a full level three structure on an abelian surface is an isomorphism of group schemes between the three torsion of the abelian surface and $(\mathbf{Z}/3\mathbf{Z})^2 \times \mu_3^2$ that preserves the Weil pairing. Nils Bruin and myself were recently able to provide new results about the geometry of the Burkhardt quartic, and the moduli interpretation of the Burkhadrt quartic.

**Result A** : It was classically known that after adjoining $\sqrt{-3}$ to the rational numbers, the Burkhardt quartic is birational to projective space. That is, there are 5 polynomials with coefficients in $\mathbf{Q}(\sqrt{-3})$ that describe a bijection between almost all of $\mathscr{B}$ and almost of all of $\mathbf{P}^4_{\mathbf{Q}(\sqrt{-3})}$. Such a map is required to have the additional property that the inverse map is also given by polynomials defined over $\mathbf{Q}(\sqrt{-3})$. By refining classical methods, Nils and myself remove the dependency on $\sqrt{-3}$. We prove that the Burkhardt quartic is birational to $\mathbf{P}^4_{\mathbf{Q}}$ by providing explicit equations for a birational map and its inverse that only involve rational numbers. As an application of the birational map, we compute the zeta function of the Burkhardt quartic.

**Result B** : The moduli interpretation of the Burkhardt quartic has been known for some time (for example see [1]), however given a sufficiently general point $\alpha = (\alpha_0 : \alpha_1 : \alpha_2 : \alpha_3 : \alpha_4)$ on $\mathscr{B}$ it was not previously clear how to write down the corresponding genus 2 curve whose jacobian realized the abelian surface corresponding to $\alpha$ explicitly in terms of the coordinates $\alpha_i$. Earlier results often required delicate computations involving certain polynomial invariants and did not take into account the field of definition of $\alpha$. With the aid of a modern computer algebra system (MAGMA) Nils Bruin and myself were able to provide a geometric method of constructing explicit family of genus 2 curves $\mathscr{C}_\alpha$, defined over the field of definition of $\alpha$, whose jacobian corresponds to the the point $\alpha \in \mathscr{B}$ for almost all such $\alpha$. Furthermore, our family contains almost all complex curves whose jacobian admits a full level 3 structure.

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# Explicit Restricted Irrationality Measures

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An irrationality measure states how well a real number can be approximated by a rational number. More concretely, given an irrational real number $\alpha$, if there exists a $\lambda > 0$ and $q_0 > 0$ such that for any $p/q \in \mathbb{Q}$ with $q \geq q_0$, if

$$\left|\alpha - \frac{p}{q}\right| > \frac{1}{q^{\lambda}}, \tag{1}$$

then $\frac{1}{q^{\lambda}}$ is an irrationality measure for $\alpha$, and we call $\lambda$ the irrationality exponent. The smaller $\lambda$ is, the less well one can approximate $\alpha$ by rational numbers. If we choose to put restrictions on the kind of rationals that we are using to approximate, this leads us to "restricted irrationality measures". An example of an explicit restricted irrationality measure is the following. Given integers $p, s$ and $k$, with $k > 12$,

$$\left|\sqrt[3]{2} - \frac{p}{s2^k}\right| > 2^{-1.62k}. \tag{2}$$

Amongst other things, these irrationality measures can be used to solve classes of Diophantine equations provided such a bound can be explicitly constructed with $\lambda$ small enough.

In this talk, I will describe the process of computing such explicit restricted irrationality measures and how they can be used to solve certain Diophantine equation. Of particular interest will be constructing restricted irrationality measures where we do not limit the denominator to a fixed power of an integer, but rather the primes involved in the factorization of the denominator come from a fixed set.

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# Improved Divisor Arithmetic for Low-Genus Hyperelliptic Curves

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The most efficient algorithms for arithmetic in the Picard group of a low-genus hyperelliptic curve are given by explicit formulas, where the group operations are expressed as an optimized sequence of field operations as opposed to arithmetic with polynomials. In this talk, we present improved explicit formulas for genus 2 imaginary hyperelliptic curves and genus 3 real hyperelliptic curves defined over finite fields. Our improvements are realized by identifying the best features of previous formulas and combining them in a novel way. In addition, we discuss on-going work on identifying families of genus 2 curves with fast $l$-tupling for $l = 2,3,5,7$.

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# Infinite Products Involving Binary Digit Sums

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The $\pm 1$ *Thue-Morse sequence* is given by

$$u_n = (-1)^{s_2(n)} \tag{1}$$

where $s_2(n)$ denotes the sum of the binary digits of the non-negative integer $n$. The following identity, originally due to Woods [8] and Robbins [7], and several of its generalisations are well-known in the literature (e.g., see Refs. [1]–[6])

$$\prod_{n=0}^{\infty} \left( \frac{2n+1}{2n+2} \right)^{u_n} = \frac{1}{\sqrt{2}}. \tag{2}$$

But no other such product involving a rational function in $n$ and the sequence $u_n$ seems to be known in closed form.

To understand such products in detail we study the function

$$f(z,w) = \prod_{n=1}^{\infty} \left( \frac{n+z}{n+w} \right)^{u_n} \tag{3}$$

We prove some analytical properties of $f$. We also obtain more identities similar to Eq. (2), such as

$$\prod_{n=0}^{\infty} \left( \frac{4n+3}{4n+1} \right)^{u_n} = 2, \tag{4}$$

$$\prod_{n=0}^{\infty} \left( \frac{(2n+2)(n+1)}{(2n+3)(n+2)} \right)^{u_n} = \frac{1}{\sqrt{2}}. \tag{5}$$

This is part of a joint work with Professors Jean-Paul Allouche and Jeffrey Shallit.

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# Multiquadratic fields of class number $2^k$

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An *n-quadratic number field*, $n \geq 0$, is any field $K$ of degree $2^n$ over $\mathbb{Q}$, which is formed by adjoining the square root of $m$ rational integers to $\mathbb{Q}$ for some $m \in \mathbb{N}$. That is, $K = \mathbb{Q}(\sqrt{a_1}, ..., \sqrt{a_m})$ for $a_1, ..., a_m \in \mathbb{Z}$ squarefree. If any of the radicands $a_1, ..., a_m$ is negative, the field is an *imaginary n-quadratic field*.

In a previous paper, F. gave a complete list of imaginary $n$-quadratic fields of class number 1 [1]. Expanding on this work, we classify all imaginary $n$-quadratic fields of class numbers 2 and 4, and extend these ideas to find a bound on the degree of imaginary $n$-quadratic fields of class number $2^k$ for $k > 2$.

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# Numerical Tests of Two Conjectures in Fake Real Quadratic Orders

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The unit group and the class group of a *real quadratic order* are the objects of two unproved but numerically extensively tested conjectures. The celebrated *Cohen-Lenstra heuristic*, widely believed to be true, asserts that the proportion of (maximal) real quadratic orders whose class number has odd part one should exist and be equal to a constant $C \approx 0.75446$. The more controversial *Ankeny-Artin-Chowla conjecture* hypothesizes that if $\Delta$ is a prime with $\Delta \equiv 1 \pmod 4$, $\mathcal{O}_\Delta$ the real quadratic order of discriminant $\Delta$, and $\varepsilon = (a+b\sqrt{\Delta})/2$ a generator of the unit group of $\mathcal{O}_\Delta$, then $\Delta \nmid b$. No counterexample exists for $\Delta < 10^{11}$; however, a heuristic argument suggests that the number of counterexamples up to some bound $X$ on $\Delta$ should grow as $0.5\big(\log\log(X) - \log\log(5)\big)$, i.e. extremely slowly. Since this value is less than 1.38 for $X = 10^{11}$, it is not surprising that no counterexample has been found.

Consider now an *imaginary quadratic order* $\mathcal{O}_\Delta$ of some fundamental discriminant $\Delta \in \mathbb{Z}^{<0}$. Let $p$ a prime that splits in $\mathcal{O}_\Delta$ and $\mathfrak{p}$ one of the two prime ideals of $\mathcal{O}_\Delta$ lying above $p$. In an unpublished note [1], Henri Cohen coined the term *fake real quadratic order* for a ring of the form $\mathcal{O}_{\Delta,p} := \mathcal{O}_\Delta[\mathfrak{p}^{-1}]$, the smallest subring of $\mathbb{Q}(\sqrt{\Delta})$ containing both $\mathcal{O}_\Delta$ and the inverse fractional ideal of $\mathfrak{p}$. The name was motivated by the surprising fact that these rings behave very much like real quadratic orders, even though they are derived from imaginary quadratic orders. In fact, a real quadratic order can be thought of as a fake real quadratic order with respect to the "prime $p = \infty$".

Fake real quadratic orders were further investigated by Richard Oh [3]. Their unit groups and class groups bear striking structural similarities to the analogues of these groups in real quadratic orders and look very different from those attached to imaginary quadratic orders. This led Cohen to pose the natural question of analogues of the two above conjectures in fake real quadratic orders, with the idea that a numerical investigation of their "$p$-versions" could potentially shed light on the validity or falsity of their original versions. Here, a major advantage is that a two-dimensional $(p,|\Delta|)$-grid yields many more data points $\mathcal{O}_{\Delta,p}$ compared to the number of quadratic orders $\mathcal{O}_\Delta$ along a $\Delta$-line. Cohen undertook modest initial computational experiments, which we extended substantially to include fundamental discriminants $\Delta < 0$ as large as $2^{40}$ in absolute value [2, 4]. Our numerical results regarding the $p$-Cohen-Lenstra heuristic were as predicted. We found that as $|\Delta|$ grows, the proportion of $\mathcal{O}_{\Delta,p}$ whose class number has odd part one approaches the same constant $C$ as above; not surprisingly, this convergence is faster for larger values of $p$. As for the $p$-Ankeny-Artin-Chowla conjecture, a few small counterexamples found earlier by Cohen could potentially have been dismissed as sporadic outliers. However, we generated millions of counterexamples; as $|\Delta|$ grows, the counterexamples thin out but do not appear to stop. Moreover, for fixed $\Delta$, the proportion of counterexamples seems to approach the expected value $1/|\Delta|$ — the probability that $\Delta$ divides a random integer $b$ — that governs the sparsity of counterexamples to the original conjecture. Our data provide convincing numerical evidence in support of the truth of the original Cohen-Lenstra heuristic, but strongly suggest that the original Ankeny-Artin-Chowla conjecture is false and the "log log" argument applies.

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# On $(a,b)$ Pairs in Random Fibonacci Sequences

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We study the random Fibonacci tree, which is an infinite binary tree with non-negative numbers at each node defined as follows. The root consists of the number 1 with a single child also the number 1. Then we define the tree recursively in the following way: if $x$ is the parent of $y$, then $y$ has two children, namely $|x-y|$ and $x+y$. This tree was studied by Benoit Rittaud [1] who proved that any pair of integers $a,b$ that are coprime occur as a parent-child pair infinitely often. We extend his results by giving tight upper and lower bounds on the number of such occurrences for any specific coprime pair $(a,b)$ at any specific level down the tree. More precisely, letting $A(n)$ denote the number of $(1,1)$ pairs $3n$ branches down the tree, we prove that

$$A(n)=\frac{243\cdot 6.75^n}{4\sqrt{3\pi}n^{3/2}}-\frac{337041\cdot 6.75^n}{288\sqrt{3\pi}n^{5/2}}+O\left(\frac{6.75^n}{n^{7/2}}\right) \tag{1}$$

with the implicit constant of the error term always lying between 0 and $\frac{1348164}{36\sqrt{3\pi}}$ for all natural numbers $n$. Also, let $A_{(a,b)}(n)$ be the number coprime pairs $(a,b)$ $3n$, $3n+1$ or $3n+2$ branches down the tree, depending on the parities of $a$ and $b$. We prove that for all coprime pairs $(a,b)$, there exists an explicitly computable positive constant $C_{(a,b)}$ and an asymptotically estimatable rational constant $D_{(a,b)}$ such that

$$A_{(a,b)}(n)=\frac{C_{(a,b)}\cdot 6.75^n}{n^{3/2}}+\frac{C_{(a,b)}D_{(a,b)}6.75^n}{n^{5/2}}+O\left(\frac{6.75^n}{n^{7/2}}\right) \tag{2}$$

where the implied constant in the error term depends upon the number of branches in the shortest path from the root $(1,1)$ to the pair $(a,b)$. In these results, 6.75 is an exact value. We also prove the following. Choose a path down the tree randomly, starting with the root $(1,1)$, with the probability of choosing a right branch be $p$ and left branch $1-p$. Then the probabiliy the path does not contain any $(1,1)$ pair except at the root is 0 if $p\leq 1/3$ and is

$$\frac{3p-2+\sqrt{4p-3p^2}}{2} \tag{3}$$

if $p>1/3$.

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# Rational Approximations of $p$-adic Algebraic Numbers and Their Conjugates

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Let $p$ be a prime number and let $|\cdot|_p$ denote the canonical $p$-adic valuation on the field of $p$-adic numbers $\mathbb{Q}_p$. The $p$-adic generalization of Roth's Theorem, established by Ridout in 1958 [1], asserts that for any algebraic number $\alpha \in \mathbb{Q}_p$ of degree $d \geq 3$ and any positive real number $\delta$ there exist only finitely many coprime integer pairs $(x,y)$ such that

$$|y\alpha - x|_p < \max\{|x|,|y|\}^{-2-\delta}. \tag{1}$$

Now suppose that $f(x) \in \mathbb{Z}[x]$ is an irreducible polynomial of degree $d \geq 5$ and content 1, and let $\varepsilon, \delta$ be positive real numbers such that $\varepsilon < 1$ and $\delta > d-4-\varepsilon$. We present computational evidence that, for all sufficiently large primes $p$, only few $p$-adic roots $\alpha$ of $f(x)$ admit a non-zero integer solution $(x,y)$ to (1). More precisely, our data enables us to conjecture that there exists a constant $p_0 = p_0(f,\varepsilon)$, such that for all primes $p \geq p_0$ the number of $p$-adic roots of $f(x)$ that admit a non-zero integer solution to (1) does not exceed some absolute constant $N$.

The conjecture made above somewhat resembles an earlier conjecture made by Stewart, which states that for a given binary form $F(x,y) \in \mathbb{Z}[x,y]$ of degree $d \geq 3$ and content 1, the number of coprime integer pairs $(x,y)$ satisfying the Thue equation $|F(x,y)| = m$ does not exceed some absolute constant $M$, as long as the integer $m$ satisfies $m \geq m_0$ for some constant $m_0 = m_0(F)$ [2]. We prove this assertion of Stewart in the case when $F(x,y)$ is a binary form of degree $d \geq 7$ with a cyclic Galois group and $m$ is a prime power. Our proof exploits the recent result of Thunder on the size of primitive solutions of Thue equations [3]. Our results can be viewed as a computational and theoretical evidence towards Stewart's conjecture.

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# On the arithmetic of a family of degree-two diagonal K3 surfaces

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Let $\mathbb{P}$ denote the weighted projective space with weights $(1,1,1,3)$ over the rationals, with coordinates $x, y, z$, and $w$; let $X_\eta$ be the generic element of the family of surfaces in $\mathbb{P}$ given by

$$X : w^2 = x^6 + y^6 + z^6 + tx^2y^2z^2. \tag{1}$$

The surface $X_\eta$ turns out to be a K3 surface over the function field $\mathbb{Q}(t)$. We will give a rough description of how to explicitly compute the geometric Picard lattice of $X_\eta$ together with its Galois module structure. This information will be used to derive some more results about the arithmetic of $X_\eta$ as well as the other elements of the family $X$.

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# Solving the *S*-unit equation in Sage

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Let $K$ be a number field and let $S$ be a set of primes in the ring of integers of $K$ including all infinite primes. Consider the equation

$$x+y=1.$$

By work of Siegel and Mahler, there are a finite number solutions in the ring of $S$-units in $K$. Baker's theorem provides a bound to the heights of these solutions, though it is extremely large[1, 2]. LLL lattice basis reduction can reduce the bound to a manageable size. Many problems in number theory and arithmetic geometry hinge on the finiteness of solutions to the $S$-unit equation, and effective, enumerative results rely on explicitly finding all solutions[5].

In 1997, N. P. Smart enumerated all genus 2 curves $C$ defined over the rationals with good reduction at all primes except $p=2$, up to rational isomorphism[7]. The most computationally difficult step was solving the $S$-unit equation. Smart went to considerable computational trouble to search for $S$-unit solutions in the fields relevant to his project. Now, this computation is easily possible on a personal computer. Inspired by Smart's work, Malmskog and Rasmussen enumerated all Picard curves with good reduction away from $p=3$[6]. In the course of this project, they implemented $S$-unit equation solving routines in Sage [4] for limited classes of fields and sets $S$. In 2014, a Sage Days 62 project group of Alejandra Avarado, Beth Malmskog, Christelle Vincent, and Mckenzie West continued the implementation project. In 2015, Angelos Koutsianas also wrote Sage code to solve the $S$-unit equation for other classes of fields and sets $S$ as part of computing all elliptic curves over certain number fields with specified primes of bad reduction. In January 2017, Alvarado, Koutisanas, Malmskog, Rasmussen, Vincent, and West all collaborated to implement a general $S$-unit equation solver for Sage. This implementation has been completed and submitted for review and incorporation into future releases. This talk will outline the theoretical basis and some practical considerations of the implementation, and discuss applications.

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# Some modular Calabi-Yau fivefolds

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Eichler and Shimura proved that, for every rational Hecke eigenform $f$ of weight 2 for $\Gamma_0(N)$, there is an elliptic curve $E_f$ over $\mathbf{Q}$ whose $L$-function coincides with that of $f$. Wiles and Taylor-Wiles famously proved the converse: the $L$-function of every elliptic curve $E$ over $\mathbf{Q}$ is attached to a modular form in this way.

The varieties whose $L$-functions should match Hecke eigenforms of higher weight are *rigid Calabi-Yau varieties*. In this talk, I will describe my work on Calabi-Yau fivefolds that are desingularizations of double covers of $\mathbf{P}^5$ branched on a union of 12 hyperplanes. We find some that do not correspond to a modular form, some for which the associated Galois representation is reducible and one component gives a modular form, and some that are rigid Calabi-Yau fivefolds.

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# The Dimensions of p-rank Strata for Cyclic Cubic Curves

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For an algebraic curve over and algebraically closed field in characteristic $p$, the $p$-part of its divisor class group is isomorphic to $f$ copies of the integers modulo $p$, where $f$ is called the p-rank of the curve. For certain families of curves, one would like to know how many curves, if any, have a given $p$-rank. To address this, we study the $p$-rank stratification of the moduli space of cyclic covers of the projective line in characteristic $p$. In particular, for all $p \equiv 2 \bmod 3$, we prove that there exists a cyclic cubic Galois cover $Y$ of the projective line, such that $Y$ has genus $g$, signature $(r,s)$, and $p$-rank $f$ for all tuples $(g,(r,s),f)$ satisfying the obvious necessary conditions. In the particular case $p = 5$, we explicitly compute enough of the low dimensional strata to prove a formula for the exact dimension of every p-rank strata for all admissible $(g,(r,s),f)$. Interestingly, our inductive proof of these results relies on proving the existence of 'balanced cuts' for all members of an infinite family of 2-coloured graphs.

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# Using Magma to study origami division polynomials

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In the theory of elliptic curves, the Galois action on the Tate module of an elliptic curve is related to the Galois group of the splitting field of the division polynomials associated to the elliptic curve. We study origami (covering curves of elliptic curves, ramified at most over one point). We define a more general notion of division polynomials for such covers. Then, we use some Galois group and invariant theory functionality from Magma to find and study these polynomials.

# SS-DAG Dynamics and Games

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# Coupling social norms and investment dynamics in a model of common pool resource harvesting

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Sustainable resource harvesting involves a tradeoff between extraction to earn revenue and conservation to promote resource replenishment. In the case of a common pool resource, this tradeoff is often interpreted as a collective action problem among a group of harvesters, who adaptively select whether to cooperate with or defect from a social norm of resource conservation. Another strand of models in ecological economics recognizes that resource harvesting can be capital-intensive, involving investment commitments that become costly to reverse if the resource is over-exploited. Working with nonlinear ordinary differential equations, we combine aspects of existing models to form a socio-ecological system. Harvesters' extractive behavior is influenced by resource abundance, social norms, and investment flexibility. We explore how model outcomes are influenced by changes to the model structure, such as the investment conditions or the social enforcement mechanisms that promote conservation.

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# Dynamic Equilibria in Decentralized Economies with Fiat Money.

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We study the dynamics of economies with decentralized markets and fiat money. The economy is populated by heterogeneous individuals that produce and trade different types goods, as exemplified in the first-generation of search model with money. To uncover the asymmetric dynamic equilibria we use a combination of analytical and computational methods. The solution algorithm is an iterative scheme over the agents' profile of trading strategies and over the evolution of assets' distribution.

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# Influence of Social Behaviour on the Evolution of Virulence

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The degree of harm a pathogen can inflict on its host is a broad definition of virulence. Virulence, depending on the investigator's perspective, can be quantified in terms of transmissibility, disease-induced death or sublethal effects on the host. Historically, social behaviour, such as social distancing or a decision to vaccinate, has proven effective in reducing the size of epidemics and in some cases eliminating a disease from a population. Mathematical models of social behaviour and their interactions with disease dynamics are increasingly used, but mathematical models of the impact of social behaviour on the virulence evolution remain little studied. We attempt to understand the influence of social behaviour on the evolution of virulence. We consider a situation where a highly virulent mutant strain is introduced to a population at an endemic state. We address the research question: Can perceived severity and efficacy of infection control prevent the invasion of the mutant strain?

We develop an evolutionary game theoretical model that couples epidemiological processes to social processes using imitation dynamics. High levels of perceived severity can drive the population to select preventive behaviour which in turn can influence the transmissibility of the disease depending on the efficacy of infection control. The system consists of 5 coupled differential equations. We perform stability analysis to draw invasion criteria. When analytical methods fail, we resort to phase planes and numerical simulations. We find that increasing perceived severity from the resident strain can, under some conditions, cause the invasion of the mutant strain. In general, when perceived severity is low, the mutant strain fails to invade for any efficacy, provided that transmission rates are equal. Similarly, when efficacy of infection control is low (in particular against the resident strain), the mutant strain also fails to invade independently from the level of perceived severity. We also find that the inclusion of social behaviour can enable the invasion of the more virulent strain, in parameter regimes for which the corresponding epidemic model without social behaviour predicts the more virulent strain cannot invade.

Emerging pathogens are of great concern in public health, so are pathogens developing drug resistance or those that evolve to be more harmful. Perhaps a big aid to public health goes beyond the production of therapeutic drugs but stems from our attitude, daily interactions and decisions. Hence, mechanistic mathematical models of the impact of social processes on virulence evolution should be further studied.

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Speaker: Ross Cressman
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Title: Interaction times change evolutionary outcomes

Abstract: Evolutionary game theory was developed under a number of simplifying assumptions. One that is not often explicitly stated is that each interaction among individuals takes the same amount of time no matter what strategies these individuals use. When interaction time is strategy-dependent, it is more realistic to take individual fitness as the payoff received per unit time. For instance, two Hawks interacting in the standard two-player Hawk-Dove game are assumed to engage in a fight, implying that they may be involved in fewer interactions than Doves who avoid such contests.

The talk will characterize how interaction times affect the game dynamics and evolutionary outcome (e.g. the evolutionarily stable strategy (ESS) and Nash equilibrium (NE)) in general two-strategy symmetric games (i.e. matrix games) and apply the results to the Hawk-Dove game. I will also show that cooperation can evolve in the repeated Prisoner's Dilemma game when the number of rounds is under the players' control. If time permits, this outcome will be related to the results from game experiments based on the corresponding opting out game.

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# Mathematical Models of Radicalization

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Radicalization is the process by which people come to adopt increasingly extreme political social or religious ideologies. In recent years radicalization has become a major concern for national security because it can lead to violent extremism. Governments and security services are making a substantial effort to better understand the radicalization process and to identify the psychological, social, economic, and political circumstances that lead to violent extremism. It is in this context that we employ compartmental epidemiological models to attempt to describe radicalization mathematically. We use these models to evaluate the effectiveness of some strategies to counter violent extremism.

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# Population Dynamics and Evolutionary Games

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This talk focuses on two-species Lotka–Volterra predator-prey and competition models in heterogeneous environments consisting of two habitat patches. Contrary to other models with passive dispersal between patches these models assume that dispersal is adaptive and it maximizes individual fitness measured by the per capita population growth rate. When fitness is frequency dependent, game theoretical approaches based on the Nash equilibrium or Evolutionarily Stable Strategies are used to define optimal animal distribution at current population densities. In this talk, I will assume that animal dispersal operates on fast time scale when compared to population dynamics. This assumption simplifies analysis of the models. I will show that for frequency independent fitness functions represented by the Lotka–Volterra predator-prey model with only predators dispersing [1], this time scale separation leads to a differential equation with discontinuous righthand side, for which solutions are defined in the Filippov sense [2]. When both prey and predators disperse, the resulting distribution is calculated as the Nash equilibrium. As interior Nash equilibria for two species are not evolutionarily stable, i.e., resistant to invasion of mutants with a different distribution, an extension of evolutionary stability [3] for two-species is needed. This extension is then used to describe distribution of two competing species among two patches. I will show how instability of the distribution can destabilize competitive dynamics that are stable at each patch [4].

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# Socio-ecological dynamics of Caribbean coral reef ecosystems and conservation opinion propagation

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The Caribbean coral reef ecosystem has experienced a long history of deterioration due to various stressors. For instance, over-fishing of parrotfish - an important grazer of macroalgae that can prevent destructive overgrowth of macroalgae - has threatened reef ecosystems in recent decades and stimulated conservation efforts such as the formation of marine protected areas. Here we develop a mathematical model of coupled human-environment interactions between reef dynamics and conservation opinion dynamics to better understand how natural and human factors interact individually and in combination to determine coral reef cover. We find that the coupling opinion and reef dynamics generates complex dynamics. For instance, the system can oscillate between low and high live coral cover as human opinion oscillates in a boom-bust cycle between complacency and concern. Under some conditions, increasing the maximum possible fishing rate can stimulate a conservationist feedback response in human populations and thus lead to greater protection of the coral reefs. In contrast, raising awareness of coral reef endangerment avoids potentially counter-productive nonlinear feedbacks and always increases and stabilizes live coral reef cover. In conclusion, an improved understanding of coral reef dynamics under anthrogenic stressors is possible using coupled human-environment models, and such models should be further researched.

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# Strategic decisions for networks of firms and buyers

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We develop a theoretical framework to study the location-price competition in a Hotelling-type network game, extending the Hotelling model, with linear transportation costs, from a line (city) to a network (town). We show the existence of a pure Nash equilibrium price if, and only if, some explicit conditions on the production costs and on the network structure hold. Furthermore, we prove that the local optimal localization of the firms are at the cross-roads of the town.

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# The optimal control of Axelrod's social norms game

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**Abstract**

In this paper, we study the well-known Axelrod's social norms game using replicator dynamics (RD) [2] and control theory [3]. The aim is to check whether using an incentive as a control parameter, Nash equilibrium strategies emerge which minimize the defecting fraction in the population. In general, a social norm game has four pure strategies: norm following, norm defecting, each of which branching further into punishing or not punishing others for defection if observed [2, 1]. By introducing a control parameter that mimics a generic incentive for players who follow the norm, we study changes in the dynamics of the game equilibria that maximize strategies that follow the social norm. We solve the control problem numerically and find that the size of incentives, as well as the capacity of individuals to observe defection by others both have an impact on the emergence of Nash equilibria in which norm following is dominant.

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# SS-DASO Data Analytics for System Optimization

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# Comparison and Analysis of Classification Algorithms for Traditional Chinese Medicine: A Case Study in Decreased Ovarian Reserve

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Objective: To conduct research on Decreased Ovarian Reserve(DOR) differentiation of Traditional Chinese Medicine(TCM) by using the technology of modern TCM diagnosis and artificial intelligence analysis method to establish the optimum syndrome classification method.

Methods: Diagnostic information of DOR patients was collected and syndromes were classified according to TCM syndrome differentiation standard. Three kinds of common data mining classification algorithm,, K-nearest neighbors， Bayesian network and support vector machine, were used for analysis on information data of the four methods of diagnosis of DOR.

Results: The time, classification accuracy, coverage rate and margin curve of establishing TCM syndrome model by the three kinds of algorithm methods under the circumstances of same training and data. The influence of the number of training samples of 3 kinds of algorithm methods was analyzed, and the model established by the three kinds of algorithms was evaluated.

Conclusion: Bayesian network algorithm is better than the other two methods in terms of the performance of DOR classification.

Key words: Decreased Ovarian Reserve(DOR); data mining; Traditional Chinese Medicine(TCM) syndrome; classification algorithm; training samples; margin curve

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# Finding Random Delay in Transit Schedule Padding

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Travel by transit is an important form of transportation. Delays in transportation can be frustrating and costly. These delays can be caused by accidents, road conditions and poor accessibility. Schedule padding refers to extra allotment of time due to these delays, but it also holds a certain amount of random delay. This research paper aims to tackle the age-old question, how can we reduce delays in transit. To evaluate, we compare the maximum real-time between two stops over an interval of stops (including known and calculated delays due to speed limits, traffic conditions and psychological limits) to the scheduled arrival (which includes padding). The difference between this is what we will refer to as the "stochastic" or random delay. After determining this "random" delay we will experiment with known parameters to address this issue and attempt to reduce delays in transit.

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# Improving the traffic jam for the SCAT-based controlling system using Q-learning method: A real case study in Iran

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## Abstract

**Traffic** congestion, rapidly increasing in many countries, has a significant impact on people's daily life. One of the most effective solutions to reduce traffic is planning the traffic lights according to the traffic volume. SCAT, one of the most commonly implemented systems around the world, is utilized in some densely populated large cities in Iran including Tehran, the capital city of Islamic Republic of Iran. To improve the performance and efficiency of such system, a method was proposed and implemented in one of the intersections of Tehran. Traffic light timings are obtained for all different hours of a day using Q-learning. Results showed proper functioning and capability of learning algorithms to reduce the traffic congestion and improvements in SCAT system.

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# Modeling with-in host dynamics of *L. monocytogenes* and understanding the dose-response relationship

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*Listeria monocytogenes* with its frequent outbreaks imposes heavy burdens on public health in North America and globally. Because of its potential threat on certain susceptible population, this food-borne pathogen is becoming a growing concern for food safety. To explore the threat *L. monocytogenes* presents to the elderly, pregnant woman and immuno-compromised individuals, many studies have focused on in-host infection mechanisms and risk evaluation in terms of dose-response outcomes. However, the connection of these two foci has received little attention, leaving risk prediction with an insufficient mechanistic basis. Consequently, there is a critical need to quantifiably link in-host infection pathways with the dose-response paradigm. To better understand these relationships, we propose a new mathematical model to describe the gastro-intestinal pathway of *L. monocytogenes* within the host. The model dynamics are shown to be sensitive to inoculation doses and exhibit bi-stability phenomena. Applying the model to guinea pigs, we show how it provides useful tools to identify key parameters and to inform critical values of these parameters that are pivotal in risk evaluation.

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# Multi-Channel Siamese LSTM for Semantic Similarity Classification

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With rapid personal content generated on Internet, application of levering such data are popular, such as question answering, machine translation, and microblog search etc. These applications mostly involve identifying similarities in natural language, especially in short text. Traditional text similarity based on tf-idf mostly failed to produce good result since word overlap are rare and sparse in such cases. Recently, distributed word representations or word embeddings have attracted a great deal of interest for learning a semantic textual similarity metric. In this paper, we investigate a range of Long Short-Term Memory (LSTM) models for representing pairs of short text, in which we learn optimal representation of sentences and a similarity function in a supervised way from labeled training data. Particularly, we propose a new Multi-Channel Siamese LSTM (MCS-LSTM) model to compare similarity with pair of short sentences. We evaluate our model on the Quora Dataset of duplicated questions, and observe significant improvements over strong basic LSTM baselines.

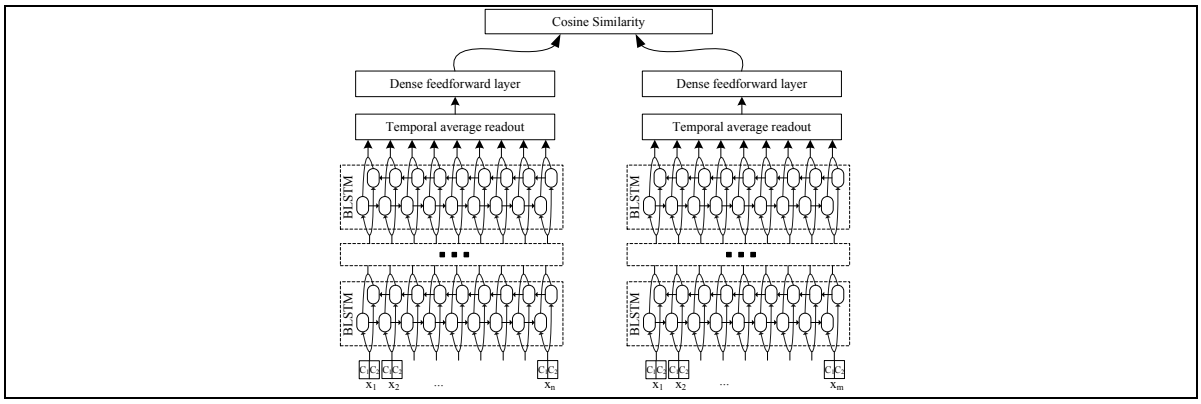


Figure 1: Multi-Channel Siamese LSTM

The aim of training is to minimize the distance in a distributed representation between similar pairs and maximize the distance between dissimilar pairs. The training data we use in the form of triplets ($x_1$, $x_2$, $y$), where $x_1$ and $x_2$ are sequences and $y \in \{0, 1\}$ indicates whether $x_1$ and $x_2$ are similar ($y = 1$) or dissimilar ($y = 0$) (e.g. "How do I read and find my YouTube comments?" and "How can I see all my Youtube comments?", is_duplicate = 1 ). In MCS-LSTM, we use a bidirectional LSMT followed by a full connect layer to encode the sentence pairs, and then use a cosine function to compute the similarity between the representation of pairs. In order to utilize rich information form, we take the word and also its part-of-speech (POS) as inputs, which is viewed as multi-channel in this paper. Our model is shown in Figure 1.

In our experiments, we use 80% of the dataset for training and 20% for testing. For the parameters of the models, we do optimization based on standard cross-validation. We compare our proposed model with both basic LSTM and Siamese models in different settings. The results are shown in Table 1.

Table1 Comparisons of Accuracy for different LSTM models

| Basic LSTM | Siamese LSTM | Multi-Channel Siamese LSTM |
|---|---|---|
| 0.7754 | 0.7912 (2.0%) | 0.8120 (4.7%) |

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# Opinion Target Extraction(OTE) model training and applying OTE to facilitate web app development

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Nowadays, people have many different considerations when they find a restaurant. However, review websites usually do not show aspects (or opinion targets). I tried to solve this problem by applying OTE findings in restaurant review web app development. Firstly, I trained an OTE model. The training of the model is a semi-supervised machine learning process: I used ixa-pipe-opinion system [1] (https://github.com/ixa-ehu/ixa-pipe-opinion) for model training. I used ixa-pipe-convert [1] to convert manually-annotated SemEval-2015 Task 12 Restaurant Train Data, Test Data and SemEval-2014 Task 4 Restaurant Train Data to CoNll 2002 format. The resultant two restaurant train data were combined to be the train set, and the resultant restaurant test data was the test set. I implemented these local features: current token and token shape (capitalization, digits, etc.) in a 2-range window, previous prediction, beginning of sentence, 4 characters in prefix and suffix, bigrams and trigrams (token and shape). I induced two types of word representations on top of them: I induced 1000 Brown [3] clusters using the implementation of Liang (https://github.com/percyliang/brown-cluster) on Yelp Restaurant Review Dataset extracted from Yelp Dataset (https://www.yelp.com/dataset_challenge/dataset) and 1000 Word2vec [2] clusters using the skip-gram algorithm (https://github.com/tmikolov/word2vec) on the Yelp Restaurant Review Dataset. Applying the trained model to perform OTE with ixa-pipe-nerc on SemEval-2015 Restaurant Test Data, the trained model has a F1 score of 96.48% calculated with the evaluation program provided in SemEval 2015 (http://alt.qcri.org/semeval2015/task12/index.php?id=data-and-tools). Secondly, I applied the trained model to perform OTE on Yelp restaurant reviews in North York, and produced a restaurant web app (https://github.com/haohao-hu/find_restaurant_app) featuring findings from the OTE: for each opinion target found, I created a HTML page showing sentences containing the opinion target automatically with a java programme. I also created an opinion target list HTML page automatically with a java programme. The webpage revealed the most commented foods in North York. The web app is based on Ruby on Rails and Bootstrap. The web app also has customer/restaurant sign up/sign in/log out and administration functionality. In conclusion, I think my study shows it is feasible and useful to apply OTE findings in website development.

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# Optimal Designs with Three factor levels and Type I Censoring for Proportional Hazards Models

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The proportional hazard (PH) model is frequently used in reliability analysis. In this paper, we focus on finding optimal design for estimating parameters and predicting hazard rate in a PH model. We consider a PH model in the form of

$$\lambda(t;\mathbf{x}) = \lambda_0(t)exp(\beta^T\mathbf{x})$$

where $\lambda_0(t)$ is assumed to be a linear baseline hazard function at the time of $t$, $\mathbf{x}$ is the column vector of covariates, and $\beta$ is a vector of unknown parameters.

We have derived Fisher information for the model parameters. We have considered three optimal design criteria. They are D- and A-optimality for estimation design and Q-optimality for prediction design. Under each optimality we have obtained both partial balanced optimal designs and unbalanced optimal designs.

In order to illustrate our method, we consider $\lambda_0(t)$ to be a simple linear function. Three types of designs (balanced optimal design, partial balanced optimal design and unbalanced optimal design) are compared.

Note that all optimal designs constructed are depending on the values of the parameters that need to be estimated. For possible misspecification in initial values of parameters, the method of construction for robust designs is also explored. We have adopted max-average design criterion which the optimal design is found to maximize the average determinant of fisher information over a given parameter space.

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# Population-Level Ambient Pollution Exposure Proxies

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The Air Health Indicator is a joint Health Canada / Environment and Climate Change Canada initiative that seeks to model the Canadian national population health risk due to acute exposure to ambient air pollution. The common model in the field [1, 2] uses averaged local ambient air pollution monitors to produce a population-level exposure proxy variable. This method is applied to ozone, nitrogen dioxide, particulate matter, and other similar air pollutants.

We examine the representative nature of these proxy averages on a large-scale Canadian data set, representing hundreds of monitors and dozens of city-level populations. The careful determination of temporal and spatial correlations between the disparate monitors allows for more precise estimation of population-level exposure, taking inspiration from the land-use regression models commonly used in geography. We conclude this work with an examination of the risk estimation differences [3] between the original, simplistic population exposure metric and our new, revised metric.

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# Ranking-based QoS Recommendation Approach

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The Quality of Service (QoS) describes how well a web service is performed, which is the measure of web service quality and availability [1]. It can help a firm to promote their services to identify services that meet their QoS requirements. As a result, how to assist service providers becomes an important problem.

Recommender systems can help users to find useful information and products. They can generate suggestions that match users' features and preferences. The recommendation systems using the Pearson coefficient predict whether a user will like an item (prediction problem). A couple of research that employ this method have been achieved as [2] [3] [4] [5] [6].

However, typical prediction generates a likeness products that would not provide an accurate score to the user. To address this issue, we propose a ranking-based recommendation using the Spearman coefficient to recommend QoS services. The Spearman coefficient is employed to calculate the similarity between the active user $a$ and user $u$. Given two rankings on a set of users, the Spearman coefficient calculates their similarity by considering the difference between the two rankings for each user. It can be computed using the following formula,

$$R(a,u) = 1 - \frac{6 \sum \ d^2}{n(n^2-1)}$$

where $n$ is the number of users, and $d$ is the difference in the two rankings for each user.

To demonstrate the effectiveness of the approach, we compare the approach using the Pearson coefficient. Results show that the approach using the Spearman coefficient can achieve more reliable rankings than the approach using the Pearson coefficient.

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# Searching Educational Resources with Ontology-based Query Expansion

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With rapid growth of Internet, a flood of educational materials is available online. However, it becomes harder for teachers to find resources which meet their specific teaching requirements and fulfill personlized satisfaction. A common problem during search is word mismatching due to language complexity. In this paper, we investegate approaches to reformulate user's query. We propose a collaborative knowledge-based approach of information retrieval for Ontario K12 education resources. In particular, we build curricula ontology(CO) and user profile ontology(UPO). Curricula are delivered by the Ontario Ministry of Education which are implied requirements of teaching content and activities for teachers. We then collectively use domain ontology (DO, e.g. mathematics domain), CO and UPO to improve query quality for better search accuracy.

The designed information retrieval system is shown in figure 1. This paper mainly focuses on ontologies construction and query expansion. The whole system is under implementation and does not finish yet. Currently we are building curricula ontologies.

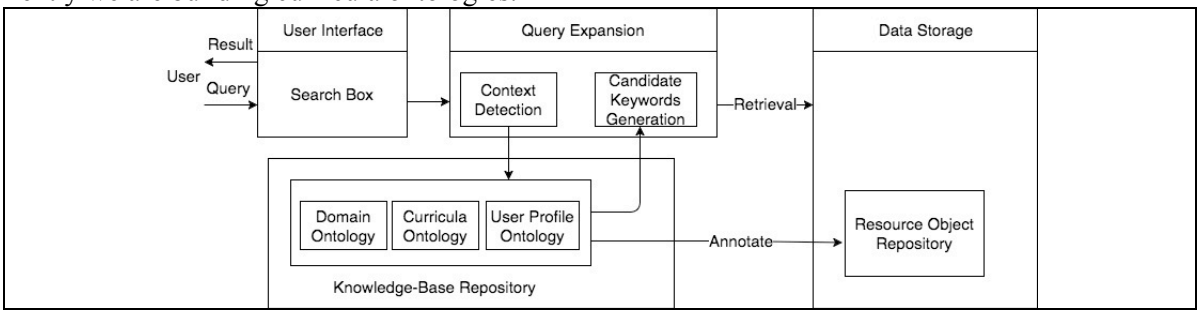


Figure 1: The flow chart of designed information retrieval process.

The significance of proposed approach is that query expansion is based on sereral ontologies. This technique can provide semantic information comparing to traditional keyword search. Hidden concepts behind keywords can be explored and utilised implicitly. It also clarifies user's intent by exploring domain knowledgy. Finally, it identifies user's seach interest, which help to implement personlization in searching process.

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# Simultaneous optimization of angles and intensities in IMRT using a new metaheuristic

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Radiotherapy is using beams to attack cancerous cells in order to eliminate them and prevent tumor growth. Although there are very accurate instruments and tools to exactly deliver desired intensity to the tumor, deciding about the angle and the intensity of the beam is a major problem. Intensity-Modulated Radiation Therapy(IMRT) is using non-uniform radiation field from given angles to the cancerous cells. Two decisions should be made here: which angles should be selected and how much intensity should each of beams have. In this study, given the multimodality of the problem, we use a new metaheuristic named Symbiotic Organism Search to simultaneously find angles and intensity of beams in order to reach the desired dose for cancerous cells while minimizing the dose received by organs at risk. in order to make a base for comparison of further researches, we used a shared data-set from literature which metaheuristics has not been applied to. For 1,3 and 5 beam(s) we found the objective function.

The problem of optimizing angles of beams according to [1] is still an open problem and in many of hospitals they still use manual selection which is error-prone, inefficient, time consuming and of course based on trial and error.

Recently [2] have used Simulate Annealing (SA) algorithm to find angles which should be used in IMRT. They mention that Beam Angle Optimization (BAO) is highly non-convex and methods based on gradient-based method would probably trap in local minimum. They used SA to solve this problem. They have not considered optimization of intensities of the beams, which we will cover in this study.

Another problem with these valuable works is that they have their own patients, no shared data set is used to know which method is better. All of these problems encouraged us to do this study and provide a base for comparison. Besides we calculate angles and intensities of each beam simultaneously.

In order to solve problems which have very vast search space and/or are highly non-convex many methods have been proposed. One of the classes are named metaheuristic. These algorithms mimic nature's behavior to solve problems. Metaheuristics algorithms, also, evolve with time. A much more recent algorithm is symbiotic organisms search (SOS). This algorithm is a very powerful metaheuristic algorithm which dominates other algorithms like PSO & GA [3].

We use this new metaheuristic to simultaneously optimize the intensities and angles of beams in IMRT using a shared dataset.

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# SS-DETA Delay Equations: Theory and Applications

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# A Periodicity Problem in a Nonlinear Differential Delay System

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We discuss a problem of existence of periodic solutions in an N-dimensional autonomous nonlinear differential system with delay. The equations of the system are cyclically coupled via delays and are of either positive or negative feedback with the overall negative feedback in the system. Typical assumptions that lead to the existence of periodic solutions are the instability of the linearized about zero system and a one-sided boundedness of one of the nonlinearities. Those are well known established facts in the lower dimensions $N = 1$ and $N = 2$. There are some results available in dimensions $N = 3$ and $N = 4$, as well as in the case of arbitrary $N > 4$. We review known results in the lower dimension and discuss their common parts and distinctions. We propose a conjecture for the existence of periodic solutions in the general case $N \geq 5$.

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# Abstraction-Based Verification and Control of Time-Delay Systems

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Abstraction-based methods [1, 3, 4, 2, 5] for verification and control of dynamical systems gained much popularity in recent years, because they they can handle nontrivial dynamics and rich specifications at the same time. Time-delay systems are infinite-dimensional systems commonly encountered in a wide range of applications. Control systems with delayed feedback are a prominent example. In many control applications, delays are inevitable and often lead to instability, loss of robustness, and undesired performance.

In this talk, we will present a computational framework that uses finite abstractions of dynamical systems for verification and control synthesis with respect to temporal logic specifications [3]. We will show that the same framework is applicable to systems described by both ordinary and delay differential equations. We will start with nonlinear dynamical systems described by ordinary differential equations and present computationally tractable procedures for abstracting nonlinear dynamics into finite-state transitions and discuss how analytical tools from dynamical system theory can provide correctness and robustness guarantees for these abstractions [4]. We show that such computational procedures are both sound and approximately complete for verification and control purposes [5]. We then extend the abstraction-based approaches to time-delay systems and show that they are effective for verification and control of time-delay systems. The results will be illustrated with several examples drawn from different application domains.

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# An alternative formulation for a distributed delayed logistic equation

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We study the alternative single species logistic distributed delay differential equation (DDE) with decay-consistent delay in growth. Population oscillation is rarely observed in nature, in contrast to the outcomes of the classical logistic DDE. In the discrete delay model proposed by Arino et al. [1], oscillating behavior is excluded. This study adapts their idea of decay-consistent delay and generalizes their model.

We established a threshold for survival and extinction: in the former case, it is confirmed using Lyapunov functionals that the population approaches delay modified carrying capacity; in the later case the extinction is proved by the fluctuation lemma. We further use the adaptive dynamics to conclude that the evolutionary trend is to make the mean delay in growth as short as possible. This confirms Hutchinson's conjecture and fits biological evidence.

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# Convergence Order of Collocation Methods for Volterra Functional Integral Equations with Non-vanishing Delays

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In this talk, we consider the numerical solution of the following general Volterra functional integral equation (VFIE) with delays

$$\begin{cases} y(t) &= g(t)+b(t)y(\theta(t))+(\mathscr{V}y)(t)+(\mathscr{V}_\theta y)(t), \quad t\in I:=(t_0,T], \\ y(t) &= \phi(t), \quad t\in I_\theta:=[\theta(t_0),t_0], \end{cases} \tag{1}$$

where the Volterra operators $\mathscr{V}$ and $\mathscr{V}_\theta$ are given by

$$(\mathscr{V}y)(t):=\int_{t_0}^{t} K_1(t,s)y(s)ds, \;\; t\in I, \tag{2}$$

and

$$(\mathscr{V}_\theta y)(t):=\int_{t_0}^{\theta(t)} K_2(t,s)y(s)ds, \;\; t\in I, \tag{3}$$

respectively. $\theta(t):=t-\tau(t)$ with $\tau(t)\geq\tau_0>0$. The kernel functions $K_1(t,s)$ and $K_2(t,s)$ in (2) and (3) are supposed to be continuous on their respective domains $D:=\{(t,s): t_0\leq s\leq t\leq T, t\in I\}$ and $D_\theta:=\{(t,s): \theta(t_0)\leq s\leq\theta(t), t\in I\}$.

We first investigate the existence, uniqueness, regularity properties, and in particular, the local representation of solutions. Based on the solution representation, we then analyze the attainable (global and local) convergence order of (iterated) collocation solutions on $\theta$-invariant meshes in detail. It turns out that collocation at the $m$ Gauss (-Legendre) points neither leads to the optimal global convergence order $m+1$, nor yields the local convergence order $2m$ on the whole interval, which is in sharp contrast to the case of the classical Volterra delay integral equations. However, if the collocation is based on the $m$ Radau II points, the local superconvergence order $2m-1$ will exhibit at all mesh points. Finally, some numerical experiments are given to confirm our theoretical findings.

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# Fliess Operators and State Dependent Time Delay Systems

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State dependent delay problem is an important problem and a hard problem. In commensurate delay case the most common and natural approach is the method of steps [1]. However, in the state dependent case the appropriate time step to use a similar approach is not obvious. Thus, it raises the question, "Does there exist the most natural sequence of time steps for a given system with state dependent time delay?". If such a sequence exists, how can one guarantee the existence and the uniqueness of the solution on each interval of the sequence? In this paper state dependent time delay system is transformed into a finite dimensional state space through a coordinate transformation. It is shown that the representation is valid locally and the time interval on which it is valid is determined. The positive time axis is partitioned into such intervals and the solution is sought for each. The existence and the uniqueness issues are addressed through the convergence of Fliess operator representation of a nonlinear system realized by a state space [2, 3]. To demonstrate our method a system with state dependent time delay of the following form is considered.

$$\dot{x} = \alpha x(t - x). \tag{1}$$

Through a coordinate transformation, this system is transformed into a state space of the following form which is valid for the $n^{th}$ time evolution step.

$$\begin{aligned} \dot{z_1} &= \alpha z_2 \\ \dot{z_2} &= \alpha z_3(1-\alpha z_2) \\ \dot{z_3} &= \alpha z_4(1-\alpha z_3)(1-\alpha z_2) \\ \vdots &= \vdots \\ \dot{z_n} &= \alpha(1-\alpha z_n)(1-\alpha z_{n-1})\dots(1-\alpha z_2)u_n(t). \end{aligned} \tag{2}$$

$$h(z) = z_1.$$

Here, $u_n(t)$ represents the state from the previous time evolution step. Then, the generating series of a Fliess operator realized by this state space can be computed by iterative Lie-derivatives of $h(z)$ with respect to the drift vector-field and the input-vector field. Existence and uniqueness of the solution is analyzed through known results from the convergence of Fliess series[3]. Also in certain cases it is found that the time evolutions steps approaches a cluster point. Both mathematical analysis and numerical simulation examples will be presented.

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# Implicit state dependent delay in range-based position estimation and navigation

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In range-based navigation, whether long base length (LBL) or single range navigation, a well known issue is that of the delay that is present between the moment of emission of a signal and the moment of reception. For fast moving units, this may pose a problem, which is addressed in this paper. Typically one solves this problem using a quasi-static assumption, i.e., that the position of the mobile units (MU) does not change significantly over the time the signal travels between the MU and the beacon (and back, in case of two-way ranging). Some works consider the MU motion to be linear and solve the problem. This paper considers the MU to be moving along an arbitrary path. We use an extension of the Lagrange-Bürman inversion to solve the problem.
Motivated by the above application we first describe the abstract problem for a system with linear dynamics

$$\dot{x} = Ax + bu \tag{1}$$
$$y = cx. \tag{2}$$

where $x$ is the state, $u$ the driving input, and $y$ a partial state. However, it is assumed that a delayed version of the partial state enters the observation equation, and that the delay is in fact a function of the partial state $y$ itself.

$$\tau(t) = By(t) + Cy(t - \tau(t)). \tag{3}$$

Typically, the delay is measured. Hence the problem is to invert Eq. (3), for which the extended Lagrange-Bürman inversion [1] is used to obtain $y(t-\tau(t))$ as an explicit function of time. Then we complement this solution with the Luenberger observer, or in the stochastic case the Kalman filter for the system Eqs. (1, 2) to obtain an estimator for the delayed state $x(t-\tau(t))$, and thus using a prediction step, also the present state $x(t)$. For $c\tau(t) = x(t-\tau(t))$, it follows with $\mathbf{D}$, the differentiation operator, and the observability condition $\dot{\beta} \neq 0$, where $\beta(t) = t - \tau(t)$, that

$$\begin{bmatrix} x \\ \mathbf{D}x \\ \mathbf{D}^2x \\ \vdots \end{bmatrix} = c \begin{bmatrix} 1 & \tau & \tau^2/2! & \cdots \\ & 1 & \tau & \cdots \\ & & 1 & \cdots \\ & & & \ddots \end{bmatrix} \begin{bmatrix} 1 & & & \\ & \mathbf{D}\beta & & \\ & \mathbf{D}^2\beta & (\mathbf{D}\beta)^2 & \\ & \vdots & & \ddots \end{bmatrix}^{-1} \begin{bmatrix} \tau \\ \mathbf{D}\tau \\ \mathbf{D}^2\tau \\ \vdots \end{bmatrix} \tag{4}$$

For instance, the 3 term series truncation yields ($c = 1$)

$$\hat{x}_{(3)}(t) = \frac{\tau}{1-\dot{\tau}} + \frac{\tau^2\ddot{\tau}}{2(1-\dot{\tau})^3} + \frac{\tau^3(\ddot{\tau}^2 + \dddot{\tau}(1-\dot{\tau}))}{6(1-\dot{\tau})^5}.$$

All hinges thus on the Lagrange-Bürman inversion which is exact in the analytic case. In order to evaluate the practical relevance, we discuss convergence issues of the developed series. If appropriate pinning conditions (exact way points) can be established this approach may provide a viable approach over traditional iterative methods. It may also be used to estimate the driving term, $u(t)$.

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# Interaction of Phage-Sensitive and Phage-Resistant Bacteria with Acquisition of Phage Sensitivity

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Phage are viruses that attack bacteria. For a lytic phage, the typical infection cycle is initiated by attachment to the host receptor, followed by injection of DNA into the host, and replication of the phage genome. After a latent period, the membrane of the host breaks down, and then the host bursts and releases mature phage.

Bacterial resistance is generally due to loss or modification of the receptor molecule to which a phage binds. Because this receptor is involved in bacterial metabolism, the resistant mutant usually suffers some cost in the form of reduced competitive ability for the limiting resource. Bohannan and Lenski [1] note that, based on experimental findings, the establishment of the resistant bacterial population does not cause extinction of the sensitive population or the extinction of phage. This prediction was confirmed by Han and Smith [2] in their mathematical model.

Recently Tzipilevich et al. [3] discovered a phenomenon called *acquisition of sensitivity*, in which bacteria lacking phage receptors can become transiently sensitive to phage and get infected. This is caused by transfer of phage receptors to the resistant cells, released from phage-sensitive cells, mediated by membrane vesicles. Acquisition of sensitivity implies that the resistant mutant loses more competitiveness than that expected in [1, 2]. In our work, we analyze a model of a chemostat with phage-sensitive and phage-resistant bacteria involving this phenomenon.

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# On linear and nonlinear equations with two delays

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We start with establishing stability properties for equations with two delays and positive and negative coefficients. Further, we proceed to nonlinear equations, where both delays can be incorporated in one nonlinear term. In particular, we illustrate how introduction of several variable delays can change properties of the Mackey-Glass equation and present some oscillation and stability-type results.

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# Stability and Periodicity in a Two-Dimensional Neural Network Model with Delay

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Sufficient conditions for the global asymptotic stability of the zero equilibrium and for the existence of periodic solutions are derived for a generalized two-dimensional neural network model with delay

$$\begin{aligned} u'(t) &= -a_1 u(t) + c_{11} f_1(u(t-\tau_{11})) + c_{12} f_2(v(t-\tau_{12})) \\ v'(t) &= -a_2 v(t) + c_{21} f_1(u(t-\tau_{21})) + c_{22} f_2(v(t-\tau_{22})). \end{aligned}$$

The results are supported with new theoretical developments and extensive numerical simulations.

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# Stability criteria of hybrid dynamical systems with distributed delays

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This paper studies a class of hybrid dynamical systems with distributed delays. Several approached are discussed in establishing stability criteria of such hybrid dynamical systems. Examples are provided to illustrate the theorems.

# SS-FCA Fractional Calculus and Applications

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# A novel approach to the discretisation of space-fractional differential equations on bounded domains

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In the last few decades, the use of fractional calculus tools has often been proposed by the mathematical community to describe transport phenomena that deviate from the classical Markovian and Gaussian paradigm. However, in order to obtain mathematical models of interest for practical applications one often has to restrict or redefine these nonlocal operators on bounded domains and provide a suitable interpretation for the role played by the boundary conditions that are imposed by the physics of the studied phenomena.

We are particularly interested in studying, on finite domains, modifications of transport differential equations in which the classical diffusive term has been replaced by some nonlocal counterpart, accounting for example for the high structural heterogeneity of the medium in which the transport phenomenon takes place.

On a bounded domain $\Omega \subset \mathbb{R}^n$, the spectral approach defines fractional powers of a nonnegative second order differential operator with discrete spectrum in terms of the eigenpairs of the operator corresponding to some prescribed boundary conditions on $\partial\Omega$. These boundary constraints are assigned *a priori*, as dictated by the physics, and determine both eigenvalues and eigenvectors of the operator on the considered domain, so that via the spectral approach one obtains a family of boundary condition dependent nonlocal operators.

Direct numerical approximation of transport equations involving space-fractional operators defined via the aforementioned spectral approach rely on explicit knowledge of the operator spectrum. If numerical computations on a finite interval and on two or three dimensional cartesian domains are pretty straightforward, the application of a direct method to real geometries is not practical, as eigenvalues and eigenfunctions are not known analytically in these cases.

Relying on the heat semi-group formalism, we propose a discretisation approach for the spectral fractional Laplacian which does not rely on explicit knowledge of the operator eigenpairs, but rather combines a suitable quadrature rule of integration with the finite element method. This approach, not only allows for a meaningful interpretation of fractional powers of the Laplacian in bounded settings but also provides a flexible strategy for their computation on multi-dimensional (possibly irregular) domains.

The same method can be used to compute fractional powers of more general second-order elliptic operators on bounded domains, accounting also for anisotropy and thus even more interesting in practical settings.

As an example of the applicability of our method we consider a simple cardiac electrophysiology model on a realistic cardiac slice geometry and show how the substitution of the classical diffusive term with a fractional counterpart affects the action potential shape and the excitation wave propagation in space.

# A second order accurate numerical approximation for time-space fractional diffusion equation

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**Abstract** Fractional differential equations arise naturally in the diffusion limit of certain random walk schemes. Anomalous diffusion in the presence or absence of an external velocity or force field has been modeled in numerous ways to incorporate the system's memory in a consistent way. It's realized that the replacement of the local time derivative in the diffusion equation by a fractional operator accounts for the memory effects which are connected with many complex systems. In this article, a numerical scheme is formulated and analyzed to solve the time-space fractional diffusion equation where the Riesz derivative is considered in spatial direction and time derivative is a fractional derivative in the Caputo form. The stability and convergence of this method are proved which shows second order accuracy both in temporal and spatial directions. Numerical experiments are also presented to verify the theoretical analysis.

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# Mixing times and relaxation to equilibrium for fractional time-changed semi-Markov processes

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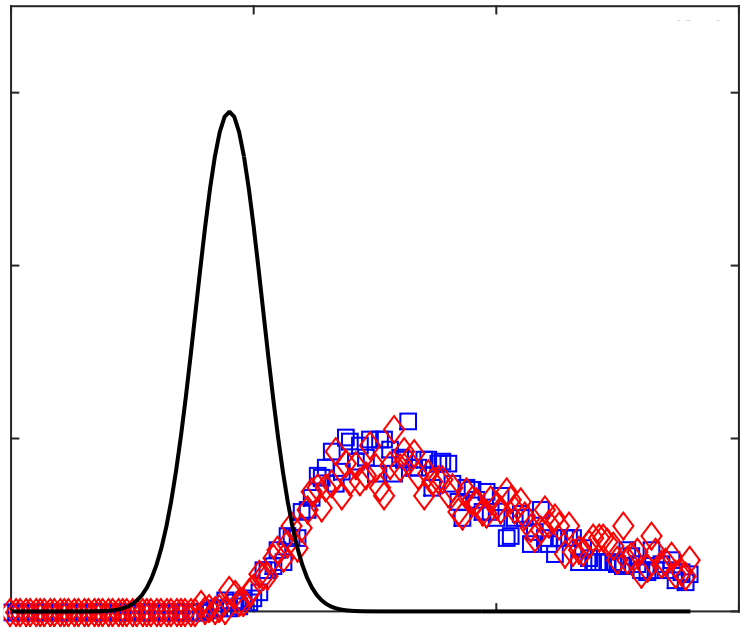
Of interest in the theory of compact space Markov processes is the relaxation to equilibrium, particularly

1. the estimation of convergence rates to the invariant measure
2. the mixing time for the chain (usually associated with reversible chains) which estimates the necessary time so that the transition probabilities and the invariant measure are close in the total variation distance.

The answer to these questions are also important when performing Monte Carlo simulations.

We are concerned with the answers to these questions when we have time-changed, continuous time semi Markov process where the inter-event times are arbitrary positive random variables with a special focus (and sharper results) on heavy-tailed (e.g. Mittag-Leffler) waiting times. Examples include semi-Markov processes on a finite and continuous compact state space.

Moreover we explore the distance between the distribution of the time-changed processes when the waiting times have the same tail exponent as a Mittag-Leffler but are not distributed like that. In the following picture you can see a comparison between a Mittag-Leffler (blue) and a Pareto (red) Ehrenfest chain.



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# Pseudo-differential relaxation equations and semi-Markov processes

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Recently, there has been renewed interest in an old result discussed by Mainardi et al. [1] that relates pseudo-differential relaxation equations and semi-Markov processes. Meerschaert and Toaldo presented a rigorous theory [2] and I recently applied these ideas to semi-Markov graph dynamics [3]. In this talk, I will present several examples and argue that further work is needed to study the solutions of pseudo-differential relaxation equations and their properties.

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# Semi-Markov models for motions in heterogeneous media

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In [4] we considered a large class of continuous time random walks (CTRWs) such that the holding time in each state has a distribution depending on the state itself. These are models of particles moving in heterogeneous media, where the trapping effect is not exercised with the same intensity at all sites. If the holding times follow an exponential distribution, then, due to the lack of memory property, the process is Markovian, otherwise it is said to be semi-Markovian.

Particular attention is devoted to the special case where the holding times have a power-law decaying density, whose exponent depends on the state itself, i.e $\psi(t) \sim t^{-1+\alpha(x)}$, $\alpha(x) \in (0,1)$. For such processes, we provide fractional (backward and forward) equations, exibiting a time-fractional derivative $\mathscr{D}_t^{\alpha(x)}$ with a position dependent order $\alpha(x) \in (0,1)$.

A suitable limit of a symmetric CTRW leads to a process governed by a variable order fractional heat equation. Such a equation has been recently derived in [1], where the authors studied anomalous diffusion in heterogeneous media. Thus our results create a further bridge between the theory of semi-Markov processes and the study subdiffusion phenomena which is a topic of statistical physics (see [3]).

In [4], our semi-Markov processes are proved to be obtained from Markov ones by replacing the physical time by the inverse hitting time of a so called inhomogeneous subordinator, such that the latter is not independent on the original Markov process (for basic information on inhomogeneous subordinators, i.e. increasing processes with independent but not stationary increments, see [5]). This result generalizes a well-known fact regarding fractional processes in homogeneous media (see for example [2]).

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# Stability and Convergence of Difference Schemes with Higher Order of Approximation for Fractional Diffusion Equation

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The time fractional diffusion equation represents a linear integro - differential equation. Its solution not always can be found analytically; therefore it is necessary to use numerical methods. However, unlike the classical case, we require information about all the previous time layers, when numerically approximating a time fractional differential equation on a certain time layer. For that reason algorithms for solving the time fractional differential equations are rather time-consuming even in one - dimensional case. Upon transition to two - dimensional and three - dimensional problems their complexity considerably increases. In this regard constructing stable difference schemes of higher order approximation is a very important task.

In the paper [1] has been found a special point for the interpolation approximation of the Caputo fractional derivative and derived a numerical differentiation $L2-1_\sigma$ formula to approximate the Caputo fractional derivative at this point with the numerical accuracy of order $3-\alpha$ uniformly. The basic properties of this difference operator are investigated and on its basis some difference schemes generating approximations of the second order in time for the time fractional diffusion equation with variable coefficients are considered. Stability of the suggested schemes and also their convergence in the grid $L_2$-norm with the rate equal to the order of the approximation error are proved.

In the case when the order of the fractional derivative is the variable $\alpha=\alpha(x)$ or $\alpha=\alpha(x,t)$ the stability and convergence of difference schemes constructed using the formula $L2-1_\sigma$ are difficult or completely impossible to prove.

In the paper [2] a new difference analog of the Caputo fractional derivative with the order of approximation $3-\alpha$, called $L1-2$ formula, is constructed. On the basis of this formula calculations of difference schemes for the time-fractional sub-diffusion equations in bounded and unbounded spatial domains and the fractional ODEs are carried out. However, until now stability and convergence of difference schemes constructed on the basis of the formula $L1-2$ remains a challenge.

In the present paper, insignificantly modified formula $L1-L2$ is proposed. The basic properties of this difference operator are investigated and on its basis difference schemes of higher order of approximation for the fractional, variable and distributed – order diffusion equation are constructed. The stability and convergence of the difference schemes are proved. The obtained results are supported by the numerical calculations carried out for some test problems.

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# The fractional non-homogeneous Poisson process

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We introduce a non-homogeneous fractional Poisson process by replacing the time variable in the fractional Poisson process of renewal type with an appropriate function of time. We characterize the resulting process by deriving its non-local governing equation. We further compute the first and second moments of the process. Eventually, we derive the distribution of arrival times. Constant reference is made to previous known results in the homogeneous case and to how they can be derived from the specialization of the non-homogeneous process.

This is joint work with N. Leonenko [1]

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# SS-FD Fair Decisions

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# An Axiomatic Approach to Cost Sharing Child Support

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We examine the problem of sharing the costs of child support between two divorced parents. In the U.S., child support is determined at the state level and different states may use different methods. However, state guidelines generally encompass similar factors to determine how much money should be allocated to raise a child. These factors include gross and net income of the parents and large expenses such as medical care, child care and special needs. The money both parents should spend to raise their child is then split between the two parents based on the type of custody agreement (dual or single-parent) and the amount of time the child spends with each parent.

Motivated by child support cost sharing rules used in Arizona and Michigan, we introduce eight interrelated axioms (Absoluteness, Weak Monotonicity, Anonymity, Complementarity, Weak Complementarity, Symmetry, Homogeneity, and Transferability) that a child support allocation function should satisfy. We provide two axiomatic characterizations of these child support functions using subsets of these axioms to prove that a child support function must have a particular functional form. We demonstrate the independence of the axioms by constructing functions that satisfy all but one of the axioms in the characterizations. The Michigan formula is part of a parameterized class of child support adjustment functions. In 2008, Michigan changed their child support function by adjusting the parameter from $k = 2$ to $k = 3$. The addition of a final axiom related to Nash's bargaining solution completes the classification of the Michigan class of such functions.

In light of these axioms, we consider the schedule used in Arizona (viewed as a step function) and the parameterized, rational polynomial function used in Michigan. Both the Michigan and Arizona functions share the same overall shape and convexity properties with maximum slope at the midpoint and minimal slopes at the endpoints. Indeed, the best-fit Michigan formula that approximates Arizona's step function has $k = 2$. We speculate about possible normative behavior based on the choice of a specific rule.

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# Catch-Up: A Rule That Makes Service Sports More Competitive

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In a game of racquetball, one player (call her $A$) serves to begin the first volley. The winner of the volley (whether $A$ or $B$) scores a point, and then serves to begin a new volley. The game continues until one player scores, say, $k = 15$ points, and so wins the game. Racquetball is an example of what we call a *Service Sport*. Other examples (with slightly varying rules) include volleyball, badminton, and squash. To estimate the first server's probability of winning the game, we assume that when $A$ serves, she wins the point with probability $p$; when $B$ serves, he wins with probability $q$; and that given the choice of servers, the points are independent events.

Let's try a new rule. What if the loser of each volley serves to the next? We call this the Catch-Up Rule (CR), and we offer it as an alternative to the Standard Rule (SR) in which the winner of each volley serves to the next.

We prove three theorems:

1. The probability that $A$ wins is the same whether we use the CR or the SR.
2. The expected length of a game is strictly longer with CR than with SR (if $p+q>1$, which is typical).
3. CR (like SR) is strategy-proof: A player's game-winning chance never improves with a lost point.

We found the first theorem surprising. A key to the proof is that with either CR or SR, player $A$ wins the game if and only if $A$ wins before her $(k+1)$-st serve. The theorems still hold when—as in volleyball—a team wins its first serve with probability $p_1$, its second serve with probability $p_2$, and so on.

We consider other rules as well, including various Trailing Rules (TR), in which the server is whichever player is behind. All of our results vary when a team needs a two-point advantage to win.

Since the CR can make games appear closer without changing the winning probabilities, it might be an attractive alternative to the SR in practice games or public competitions. We would love to hear about experiments!

**Comparing direct algorithms for two-player fair division of indivisible items: A computational study**

by D. Marc Kilgour and Rudolf Vetschera

**Abstract**

We present an exhaustive computational study of algorithms for two-person allocation of indivisible objects. We identify eight algorithms that generate balanced allocations using only players' ordinal rankings and test them over all possible rankings of up to $N = 12$ items. Algorithms are evaluated according to the fairness and efficiency properties of the allocations they produce, including the ordinal properties of envy-freeness, Pareto-optimality, maximinality, and three similar properties based on Borda count. Our results indicate that, overall, the algorithms manage to identify a large majority of allocations that exhibit all three of the ordinal properties. Algorithms that combine bottom-up and top-down approaches find at least one good allocation whenever one exists, while other algorithms fail sometimes. Performance is not as good for Borda properties: In about 6.6% of the problems in which such an allocation exists, no algorithm can find it. We provide examples that illustrate how algorithms behave, and how they fail. We also discuss the overlap between allocations found by different algorithms, and find that algorithms combining both directions are able to find most of the allocations found by unidirectional algorithms, although there are many instances of allocations that can be found only by an algorithm in the latter group.

**Continuity and Incentive Compatibility in Cardinal Voting Mechanisms**

by

Lars Ehlers, Dipjyoti Majumdar, Debasis Mishra, and, Arunava Sen

# 1 Extended Abstract

Many important models in mechanism design preclude the use of monetary transfers. This may be due to ethical (school choice problems, kidney exchange problems) or institutional (voting) reasons. A typical model in such an environment consists of a set of alternatives and ordinal preferences (strict linear orders) of agents over these alternatives. A mechanism or a social choice function (scf) selects a lottery over the set of alternatives. A notable feature of these models is that they only use ordinal information about preferences over alternatives. In this paper, we ask if there is any loss of generality in restricting attention to ordinal mechanisms in such environments.

Casual reasoning suggests that a mechanism that uses "a lot of" information regarding agents' preferences is more susceptible to manipulation by agents. Two well-known results in this literature are illustrations of this informal principle. If all preferences are admissible, the Gibbard-Satterthwaite Theorem (Gibbard (1973), Satterthwaite (1975)) states that the only information that an incentive compatible mechanism can use, is the preference information of a *single* (dictator) agent. If preferences are single-peaked, only *peaks* of agent preferences can be used in computing the social outcome at a profile (Moulin (1983)). Our results accord with this principle. Although cardinal information is available, we show that incentive compatibility in (private values) voting models implies that most of it cannot be used by the designer.

If the solution concept is dominant strategy and the mechanism is deterministic (i.e., lotteries produced by the scf are degenerate), then incentive compatibility immediately implies that the scf cannot be sensitive to cardinal information. However, the answer to this question is not obvious if either (a) we allow for randomization and/or (b) we use the weaker solution concept of Bayesian incentive compatibility. It seems natural therefore to believe that this cardinal preference information can be used by the mechanism designer to determine the value of the scf at various profiles.

Our main result shows this to be false. We establish that every dominant strategy incentive compatible, cardinal and random scf that satisfies some version of continuity, is ordinal. We discuss two notions of ordinality and, correspondingly, two notions of continuity.

Our first notion of ordinality requires that we treat two utility vectors representing the

same ordinal ranking over *lotteries* in the same manner. In other words, we say that an scf is *vNM-ordinal* if $u_i$ and $u_i'$ are two utility vectors which are affine transformations of each other, then the outcome of the scf is the same at $(u_i, u_{-i})$ and $(u_i', u_{-i})$.

Our second notion of ordinality, which we call *strong ordinality*, requires that the scf be sensitive to only ordinal ranking of *alternatives*. In other words, strong ordinality says that if $u_i$ and $u_i'$ are two utility vectors which represent the same ordinal ranking over alternatives, then the outcome of the scf is the same at $(u_i, u_{-i})$ and $(u_i', u_{-i})$. Strong ordinality implies vNM-ordinality because if $u_i$ and $u_i'$ are affine transformations of each other, then they represent the same ordinal ranking over alternatives.

We impose two versions of continuity. Fix the types of all agents except an arbitrary agent $i$. If $i$ varies the cardinal intensities of her preferences over alternatives without changing her ordinal ranking over the alternatives, then the outcome of the scf must vary continuously. Our notion of continuity is clearly weaker than the standard notion in that it applies only to subdomains where the ordinal rankings over alternatives are unchanged. Thus, our formulation allows scfs to be sensitive to cardinal intensities but restricts them to be continuous in a limited sense. We call this requirement *cone continuity (c-continuity)*. We also consider a stronger version of continuity where we require the outcome of the scf to vary *uniformly* continuously. We call this requirement *uc-continuity*. Our main result shows that every dominant strategy incentive compatible scf is vNM-ordinal *almost everywhere*. In other words, there is a dense subset of the domain where the scf is vNM-ordinal and the complement of this subset has measure zero. We give an example to illustrate that dominant strategy incentive compatibility does not imply vNM-ordinality (everywhere) - this is in contrast to the trivial conclusion in the deterministic scf case, where incentive compatibility implies (strong) ordinality. We use our main result to establish two striking results: (a) every c-continuous and dominant strategy incentive compatible scf is vNM-ordinal and (b) every uc-continuous and dominant strategy incentive compatible scf is strongly ordinal. We emphasize here that incentive compatibility itself implies c-contunuity of the scf almost everywhere. Our assumption implies that if we strengthen it to everywhere, we get vNM-ordinal scfs. Further, if we strengthen it to uc-continuity everywhere, we get strongly ordinal scfs.

Cycles and intractability in social dichotomy and trichotomy rules

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A dichotomy T > B partitions a set into top and bottom subgroups – job applicants who make an initial cut, and those who do not, for example. The ***Mean Rule*** of Duddy and Piggins aggregates individual dichotomies (those recommended by individuals on a hiring committee, perhaps) into a collective dichotomy. Its normative appeal is that it minimizes the differences between pairs of candidates within a common subgroups, as summed over all such pairs and all committee members, and this collective dichotomy can be calculated easily. We can easily generalize the Mean Rule to obtain a method for aggregating trichotomies, with similar normative appeal. But computing the collective trichotomy turns out to be an NP-complete problem.

What makes the difference? We show that these rules, along with a host of others (the Borda count and Approval voting rules, for instance) are special cases of a recent generalization of the Kemeny voting rule. An analysis of the orthogonal decomposition of a tournament into cyclic and cocyclic components then reveals that computational complexity arises from the cyclic component, explaining why some of these special cases are easy to compute while others are intractable.

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# Fair Assignments for Generalized Tennis Problems

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A group of friends organize their tennis games by submitting each their availability over the weekdays. They want to obtain an assignment such that each game must be a double tennis match, i.e. requires four people, and nobody plays in a day he is unavailable. Can we construct assignments that are efficient and fair? And if so, how? We use tennis scheduling as a motivation, but our problems includes the assignment of courses to students, food to charities, and of individuals to committees.

In this tennis assignment problem, that we describe formally in the paper, players have dichotomous preferences over the days they play: either they want to play on a given day or they do not. These preferences were first studied by [1] in the context of assignment problems, and the preferences here represent a natural extension of those: agents want to play in as many feasible days as possible, so players' preferences can be described as a subset of days. Any assignment that makes them play on a day they are not available is just not feasible. The constraint that 4 people are required to create a game has been previously imposed by [3] over assignments with one day only. Our model is a natural generalization of Shubik's problem on the domain of dichotomous preferences.

This problem differs from the standard fair division setup because the number of goods to be assigned depends on the players' preferences. Whereas efficiency, fairness, and non-manipulability can be achieved in the domain of dichotomous preferences, two standard results disappear: the egalitarian solution cannot be supported by competitive prices, so it can no longer be computed with the Eisenberg-Gale program maximizing the Nash product, and the competitive allocation with equal incomes is no longer unique.

Both results are surprising. In [1], the egalitarian solution is always supported by competitive prices. The fact that the competitive solution is not unique is surprising as uniqueness always obtains in Fisher markets, see [4]. The multiplicity of the competitive solution allows for manipulation both by the players and the mechanism designer.

Introducing a new fairness axiom, we identify a third solution that presents an appealing compromise between egalitarianism and market decentralization, at the cost of not preserving the group strategy-proofness of the egalitarian solution. Both solutions are Lorenz-dominant for two sets of feasible utility profiles.

Most of our results apply to the course allocation problem [2].

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# Fairness, Voting, and Symmetry

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At a fundamental level, fairness appears in discussions about voting when we require voting procedures to treat all candidates the same way. Fortunately, such requirements can often be encoded as well-understood symmetry requirements of simple mathematical functions. Interestingly, these symmetry requirements do more than help us make sense of basic fairness requirements—they also lead to new questions and techniques in voting theory.

In this presentation, I will explain how the mathematics of symmetry can be used to great effect in the study of voting. In particular, I will discuss how some of the results found in papers such as [1, 3] were proved using elementary ideas from the representation theory of symmetric groups. I will also discuss how such ideas can be used to better understand foundational results and promising generalizations in cooperative game theory [2].

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# Identifying top researchers with respect to multiple aspects of centrality

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Quantifying the importance of entities and identifying the most important one in a system are of interest in many studies. Opsahl, Agneessens, & Skvoretz used Freeman's EIES dataset to analyze the importance of 32 researchers who collaborated on several projects in the field of Social Network Analysis in 1978 [1]. They represented the data as a network, where the researchers are the nodes and there is a link between two researchers if they communicated by sending at least one message. Then, the authors measured the number of communication partners of a researcher by the *out-degree centrality* and the number of messages sent by a researcher using the *out-strength* measure. By determining the relative importance of two measures, they identified top researchers. The question then arises: what if one or two measures are not enough to fairly characterize the importance of a person?. To address this question we obtain the number of citations for researchers as an additional feature that nonetheless describes a person's importance in a field. This refers to a Multi-Criteria Decision Making problem. In order to solve it we use a well-known fuzzy operator (Ordered Weighted Averaging) [2]. Using the proposed approach, we visualize how the different values of a parameter change the rankings of researchers as it produces different decision strategies.

**OWA**: Let $A$ be a vector of values for multiple criteria and let $B$ be a non-increasingly sorted version of it. The OWA operator is then equated by Yager using Eqs. (1, 2).

$$\lambda_{OWA}(a_1, a_2, \cdots, a_m) = \sum_{j=1}^{m} w_j b_j, \qquad (1)$$

$$w_i = \left(\frac{i}{m}\right)^{\beta} - \left(\frac{i-1}{m}\right)^{\beta} \text{ for } i = 1, \cdots, m \quad (2)$$

where $\beta \geq 0$ and the OWA weights satisfy the conditions of $\sum_i w_i = 1$ and $w_i \in [0,1]$. If $\beta = 0$, the weight vector $W$ is $[1,0,\cdots,0]$ (*OR* aggregation). If $\beta = 1$, all values of $W$ are $1/m$ (averaging) and if $\lim_{\beta \to \infty}$, $W = [0,\cdots,0,1]$ (*AND* aggregation). For each numerical vector of $a^j$, a normalization is performed by computing $a'^j[i] = \frac{a^j[i] - \min}{\max - \min}$, thus all the values of $A$ are between 0 and 1.

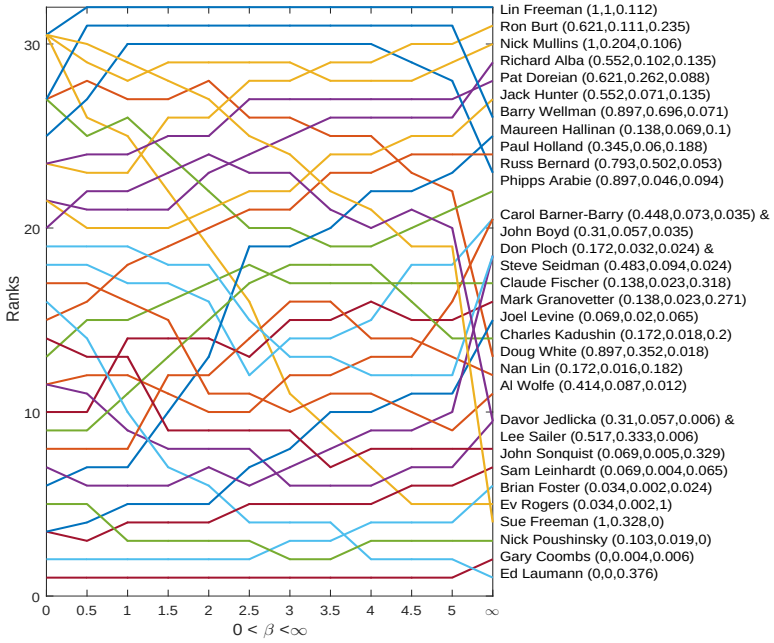


Figure 1: The ranking of 32 researchers with respect to the different aggregation strategies (guided by $\beta$) over three criteria respectively: (# of communication partners, # of sent messages, # of citations).

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# Measuring Discord from Preferences Over Indivisible Items

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Consider the situation where two parties partition a set of $2k$ indivisible items into two sets of $k$ items each. We require each party to strictly rank all items from most to least preferred. For a given allocation, each party's satisfaction can be measured using the respective ranking. If one party's ranking is used to label the items, so that one ranking is $1, 2, \ldots, 2k$, then the other party's ranking can be considered as a permutation $\pi \in S_{2k}$.

There are various algorithms in the literature for optimal ways to produce allocations, varying by the sequence of selection and whether preferences are publicly known, where optimality can be measured by several notions of fairness (e.g., [1, 2, 3]). Some algorithms make use of a "contested pile" (CP) of items not initially allocated to either party; there is subsequent literature on how to deal with these items. Most thorough treatments consider all possible preferences, i.e., all $\pi \in S_{2k}$, while acknowledging that these are not equally likely:

> If one assumes that [the second player's] order is chosen at random from $S_{2k}$, then we have the pleasant conclusion that both players are guaranteed their worst outcomes with probability $\frac{1}{(2k)!}$ while they both get their best outcomes much more often, with probability $\frac{(k!)^2}{(2k)!} = 1/\binom{2k}{k}$, the inverse of a central binomial coefficient. This may be a valid assumption for the example of colored bowls, since color preferences might be independent. In the NFL draft, however, it is likely that every team values the Heisman Trophy winner highly, for instance. Any positive correlation between the players' preferences skews these probabilities toward discord. [2, p. 293]

> But equiprobability is not a realistic assumption in most real-life situations, wherein the players' preferences are correlated. How the degree of correlation affects the proportion of items that are allocated to the players—versus those that go into CP—remains to be investigated. [1, p. 140]

Our goal is to develop a useful measure of the correlation mentioned in the quotations.

Certainly there are many metrics for permutations in algebraic combinatorics, but they do not address the particularities of the allocation application. For instance, the rank of a permutation $\pi$ can be determined by writing $\pi$ as a minimal product of transpositions (permutations that swap two items). However, a transposition involving a small number (e.g., an item highly values by at least one player) will generally have a larger impact on allocations than a transposition involving two large numbers (items of low rank for at least one player). The $C(k)$ conditions of [1] are a helpful ingredient.

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Under the National Popular Vote (NPV) plan, states join an interstate compact and pledge to cast all their electoral votes for the national popular-vote winner. NPV becomes law only after states with a majority of electoral votes enact it, which would ensure the election of the popular-vote winner. So far, states having almost half the votes needed for NPV to become law have passed NPV. We propose a Modified Popular Vote (MPV) plan whereby states, independent of what other states do, pledge to cast all their electoral votes for the national popular vote winner. This measure would benefit the 41 states in the 2012 presidential election that received virtually no attention from the candidates because they were not considered competitive. Voters in these states would increase their Banzhaf voting power by up to half what they would have if they were competitive. Prospects for the adoption of MPV are briefly discussed.

# SS-GLS Geocomputational Landscapes and Spaces

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# Alternative spatial foundations for GISci.

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If we take seriously the fact that we almost always work in discrete spaces in GISci.. Why do continue to use tools that assume a continuous underlying space? In this paper we review the important issues raised by Stell and Webster [3] in this problem domain and offer a brief glimpse at a research program that provides alternative foundations for robust computing for GISci..

We discuss first how certain key topological theories, such as Jordon's curve theorem and Kelly's theorem, break down when we move from a continuous to a discrete space [3]. Next we provide a sketch of some earlier attempts, such as those by Schneider [2], address these foundational issues. Finally we introduce and expand upon Stell and Webster's oriented matroid proposal by incorporating ideas introduced by Bokowski [1], Ziegler [4], and others that utilize the chirotope sign vector representation of the signed bases of point patterns as a basis for the analysis of their convexity and intersection properties, two of the main spatial analytic components at the base of GISci..

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# Determining Lichen volume in the Bathurst Caribou winter range using high resolution UAV and Landsat imagery

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## Abstract

The Bathurst Caribou Herd has experienced a ~95% population decline since 1996. Many northern barren ground caribou herds have experienced similar declines. Population cycles naturally occur within large caribou herds; however, these numbers are alarmingly lower than prior years. It is hypothesized that the cause of this decline is linked to food availably during the winter months. Ground lichen make up a major component of caribou caloric intake in the winter. Understanding of the spatial extent and distribution of lichen throughout the winter range is therefore a pressing information need. The objective of this paper is to use a recently developed lichen volume estimator (LVE) to determine the volume of lichen in the winter range of the Bathurst Caribou Herd. The LVE can be derived from Landsat imagery to detect presence of ground lichen and indicate the volume of lichen within each 30m pixel. However, the provenance of the LVE in the Canadian Low Tundra is unknown. A multi-scale hierarchical validation procedure was developed to validate the LVE comprising very-high resolution imagery obtained from unmanned aerial systems, and georeferenced field photographs for 13 sites in August 2016 at the Tundra Ecosystem Research Station located on Daring Lake, NWT. Ecognition was used to classify the ground lichen for both the UAV and georeferenced photographs collected for ground truthing. It is thought that the results from this paper can be broadly used to develop energy expenditure models as well as assist in determining regions suitable for habitat protection.

## Keywords

Bathurst Caribou Herd, Lichen, Remote Sensing, UAV

# Distributed Snow Simulations for Quantification of Snow Accumulation Across an Arctic Shrub-tundra Landscape

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**Abstract**

Arctic environment is characterized by an uneven distribution of snow, which is a result of snow erosion and transport and deposition (drift). The vegetation and the topography control the redistribution of water storage in different land features of the arctic environment. Wind redistribution of snow involves erosion of snow cover, transport of the blowing snow from exposed areas, and deposition snow on lee sides of hill and tall vegetation or other obstructions. Vegetation height and cover pattern influence the spatial distribution of the snow which in turn, affects the vegetation growth and distribution. The heterogeneous distribution of snow in these regions often occur at a scale less than 0.5 to greater than 5-m deep snow within a

horizontal distance of 100 m. In this study, we evaluated the performance of a distributed 10-m high resolution snow model with wind-induced snow transport capability (SnowModel) by comparing the model estimates of snow accumulation and redistribution with in situ snow observations made over three subdomains within the Trail Valley Creek drainage basin located approximately 50 km north-northeast of Inuvik, NT, Canada. The subdomains have various topographic complexity, vegetation composition and spatial extent. SnowModel was run from October 1, 2012 to May 31, 2013. In situ snow surveys were conducted in December 2012, March and April 2013. We will present the performance of the model as a function of vegetation types and landforms and outline its limitations and areas where further research is needed.

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# Spectral-temporal modelling of bamboo-dominated forest succession in the Atlantic forest of southern Brazil

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With access to collections of continuous satellite imagery over a 40-year period, spectral-temporal patterns extracted from multi-temporal imagery offer a potential new tool to monitor changes in forested landscapes. Specifically, spectral-temporal trajectories associated with successional forest change occurring over long time periods may enhance periodic 'snapshot' classification methods that ignore time. In this paper, Landsat-time series are used to examine the spectral-temporal signatures of bamboo-dominated forest succession occurring within the critically threatened Araucaria Forest, a pine-dominated subtype of the Atlantic Forest in southern Brazil. Alteration of canopy structure through ongoing anthropogenic disturbance has increased understorey light climate and given opportunity for native invasive bamboos to flourish, resulting in drastic reduction of tree regeneration and loss of biodiversity. We aimed to evaluate how spectral-temporal signatures could be used to (1) characterize stages of bamboo-dominated forest succession and (2) classify regions of bamboo-dominance. First, a theoretical spectral-temporal model was developed and compared to a 32-year Landsat time-series of vegetation indices by calculating root-mean square error between each pixel in the study area and the model. Subsequently, a time-weighted dynamic-time warping classification approach was used to classify regions of bamboo-dominated forest. It was found that spectral-temporal patterns aided in characterizing stages of bamboo-dominated forest succession and the developed theoretical spectral-temporal model proficiently classified regions of bamboo-dominance, achieving between 77% and 90% accuracy. To compare classification performance between 'snapshot' and multi-temporal imagery classification methods, a maximum-likelihood classification was performed, which attained lower overall accuracies between 70% and 83%. The dynamic model had lower overall accuracy than both methods (68% to 82%), but is still considered a useful tool for automated classification purposes that take advantage of multi-temporal imagery.

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# The prevalence and use of relative spatial expressions to denote location by online news articles

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Geographic information retrieval has advanced considerably in the last decade, enabling translation of spatial language embedded in text to machine-readable data supporting search engine queries and mapping tools. However, while considerable inroads have been made in toponym extraction and disambiguation, relative spatial language continues to be a key research frontier. Expressions such as prepositions, adverbial phrases, or surrogate expressions with spatial meaning (e.g. in the centre of, at, down the street from) are difficult to extract and structure [1].

This study will take an exploratory approach to the use of spatial language in online news articles. We will examine the frequency and type of spatial expressions in online news reports with a focus on the prevalence of absolute spatial expressions (e.g. toponyms) denoting location and relative spatial expressions or locations specified with relative spatial expressions referenced from a given absolute spatial expression (e.g. the farm on the outskirts of Toronto). A typology of 'spatial anchoring' mechanisms is proposed based on the above analysis of a sample of 500 articles obtained from online news sources. As well, the study will look at differences in the articles' themes, such as a comparison of local and national news sources, to evaluate different approaches to spatial anchoring. Unsupervised classification will categorize the different uses of both absolute and relative spatial anchoring within the documents to elicit possible connections to how and when they are used, such as possible use of more relative spatial expressions when the targeted population of the information is local, and therefore more spatially knowledgeable of the location.

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# Using High-frequency Coastal Radars for Calibration of AIS Based Ocean Vessel Tracking Models

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Most of the world relies on ships for transportation of cargo and people. Automatic Identification System messages are transmitted from ships and provide a wealth of positional data on these open ocean vessels. This data is being utilized to determine the optimal path for ships as well as predicting where a ship may be going in the immediate future [1]. It has only been in the past decade that Automatic Identification Systems signals have been easily received with satellites so there have been few studies that look at using available information and pairing it with the new abundance of ship positional data.

Previously established systems and datasets can be paired with the Automatic Identification data to help develop ship prediction models. One of these established systems is the high frequency radar data network that tracks the velocity of surface ocean currents off of the West Coast of North America. Networks of high frequency radars are located on coasts around the world and measure wave velocities up to 200km from the coast[2, 3]. These near real time measurements allow for wave velocity data to be paired with near real time Automatic Identification System messages.

The aim of this study is to explore the relationship between error in a prediction model and wave velocities derived from coastal high frequency radar signals. This study creates a model that predicts a ship's location and calculates the error from that prediction. These errors are compared to corresponding high frequency radar data to detect a statistical relationship between the displacement and prevalent waves. The high frequency data can then potentially be incorporated back into the model as a calibration to predict a ship's future location.

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# SS-GMCTA Geometric Mechanics and Control: From Theory to Applications

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# A variational Lagrangian formulation for nonequilibrium thermodynamics

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We present a Lagrangian variational formulation for nonequilibrium thermodynamics. This formulation extends the Hamilton principle of classical mechanics to include irreversible processes in both discrete and continuum systems. The irreversibility is encoded into a nonlinear nonholonomic constraint given by the expression of entropy production associated to the irreversible processes involved. The introduction of the concept of thermodynamic displacement allows the definition of a corresponding variational constraint. We also present the geometric structures underlying nonequilibrium thermodynamics. We illustrate our theory with both finite and infinite dimensional examples, including mechanical systems with friction, chemical reactions, electric circuits, and multicomponent reacting fluids.

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# Abstract numerical analysis

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> *Their studies until that point in time would have consisted, to a large extent, of a progression of formal reasoning, the familiar sequence of axiom ⇒ theorem ⇒ proof ⇒ corollary ⇒ ….. Numerical analysis does not easily fit into this straitjacket, and this goes a long way toward explaining why many students of mathematics find it so unattractive.*
>
> *Arieh Iserles*

The numerical analysis of ordinary differential equations occurs, for the most part, in the setting of open subsets of $R^n$. This is natural because in the machine implementations almost everything is anyway a tuple of floating point numbers. As a result, though, Euclidean space overbears in the theory. The convenient and familar structures of $R^n$ lead to constructs that are not deeply natural, and to immaturely architected mathematics. A formal definition of a numerical method with values in a *topological space* will be presented, leading to a better architected development of the numerical analysis of ordinary differential equations. The generality is such that the continuous and discrete theories of differential equations become unified.

The basic definition can be motivated by considering what it means for a discrete approximation $y_{h,k}$ to converge to a solution $y(t)$ of an ordinary differential equation. Most natural would be something like pointwise convergence, i.e.,

$$\lim_{h\to 0^+} y_h(t) = y(t), \qquad t \in \text{domain}(y), \tag{1}$$

where $y_h$ is the (partial) function defined to have values $y_{h,k}$ at $t_{h,k} \equiv kh$. Of course this is not possible because the $y_h$ are not defined at every $t$ for which $y(t)$ is defined. So, in the general practice [2, 4], convergence means something more like

$$\lim_{h\to 0^+} \max_{k=0,1,\ldots,\lfloor t^*/h \rfloor} \|y_{h,k} - y(t_{h,k})\| = 0. \tag{2}$$

Expendiently, the smooth solution has been evaluated at varying times dictated by the domains of the approximations, and the Euclidean norm used to compare the differences. This would have been inhibited had there been no norm in the first place, and then the following would have been more visible: a sequence of mesh functions $y_n$ converges to a solution $y$ if

$$\text{for all } t \in \text{domain}(y),\ \lim_{n\to\infty} y_n(t_n) = y(t) \text{ whenever } t_n \in \text{domain}(y_n) \text{ and } t_n \to t, \tag{3}$$

which is more-or-less equivalent to the well-known compact-open topology. There is a substantial literature about topologies of spaces of partial functions and the related hyperspace topologies of subsets of a topological space, which is not based on norms nor distance functions [1, 3]. An *abstract (numerical) method* will be defined as a covering by collections of continuous partial functions between topological spaces, with topology arranged so that convergence is aligned with (3).

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# Dynamics of Solar Sailing

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Solar sails are a form of spacecraft propulsion using solar radiation pressure. Solar sail spacecrafts are propelled by the impact of the photons emitted by the Sun against highly reflective membranes of the sail, providing a free and nearly limitless source of energy. Though acceleration is initially slow, it is continuous, giving a solar sail spacecraft the ability to reach very high velocities, and undertake long term missions that conventional craft cannot. A potential future mission is the Geostorm Warning mission ([1]), where a sail is to be placed sunwards of the Earth-Sun $L_1$ point (Lagrange points ($L$-points) are the equilibrium points found in the vicinity of the two orbiting masses). With a magnetometer the solar wind polarity can be detected giving enhanced warning of the geomagnetic storms, doubling the time of alert of a conventional $L_1$ Halo orbiter such as the Solar and Heliospheric Observatory (SOHO).

In this project, the Restricted Three Body Problem (RTBP) is considered ([1]) taking Earth and Sun as primaries and adding the solar radiation pressure, to describe the motion of a solar sail spacecraft in the Earth-Sun system. The sail orientation is parametrized by two angles: $\alpha$, the angle between the Sun-line and the projection on the ecliptic plane of the normal vector to the sail, and $\delta$, the angle between the ecliptic plane and the normal vector to the sail. Another parameter, $\beta$, represents the sail lightness number. With these we find a 2D family of artificial equilibria parameterised by the sail orientation. It can be shown that most of these points are unstable. These artificial equilibria are possible targets for the Geostorm mission and other future missions. The control of these equilibria is of great importance for Geostorm. We show that station keeping of a solar sail spacecraft near an unstable equilibrium point can be achieved by adjusting the sail orientation to keep the trajectory of the spacecraft close to the equilibrium point.

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*Title*: **Exact geometric approach to the discretization of fluid-structure interactions**

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*Abstract*: Variational integrators for numerical simulations of Lagrangian systems have the advantage of conserving the momenta up to machine precision, independent of the time step. While the theory of variational integrators for mechanical systems is well developed, there are obstacles in direct applications of these integrators to systems involving fluid-structure interactions. In this talk, we derive a variational integrator for a particular type of fluid-structure interactions, namely, simulating the dynamics of a bendable tube conveying ideal fluid that can change its cross-section (collapsible tube). We deriving a fully three-dimensional, geometrically exact theory for flexible tubes conveying fluid. Our approach is based on the symmetry-reduced, exact geometric description for elastic rods, coupled with the fluid transport and subject to the volume conservation constraint for the fluid. Using these methods, we obtain the fully three dimensional equations of motion. Based on this theory, we derive a variational discretization of the dynamics based on the approximation of the fluid's back-to-labels map, coupled with a variational discretization of elastic part of the Lagrangian. We also show the results of simulations of the system with the discretization using a very small number of spatial points demonstrating a non-trivial and interesting behavior. Time permitting, we shall also discuss the applications of our methods to the case of the flow of compressible gas and tubes with elastic walls.

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# Motion in a Symmetric Potential on the Hyperbolic Plane

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We study the motion of a particle in the hyperbolic plane (embedded in Minkowski space), under the action of a symmetric potential. This problem can be viewed as an extension of the spherical pendulum in the gravitational force field. In the case under consideration, however, one has to distinguish three inequivalent cases, depending on the direction of the force field. Symmetry reduction, with respect to groups that are not necessarily compact or even reductive, is carried out by way of Poisson varieties and Hilbert maps. We will discuss the dynamics of the system in the case of linear potentials.

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# On the Hamiltonian equations for the coupled system of a free surface and a rigid body

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The dynamics of free surfaces and water waves is a classical topic in fluid mechanics. The dynamics of solid objects on and below these surfaces has also been well-investigated. Typically, however, most investigations for the body+fluid system use linearized approaches or prescribed dynamics for the body or the fluid. Little attention seems to have been paid to the fully coupled and nonlinear dynamics of a free surface and a rigid body close to the surface. In particular, the scientific literature on the Hamiltonian formalism for the coupled system in an inviscid setting is quite sparse. The talk will first introduce the Poisson brackets for such a system in a spatially-fixed frame Refs. [1]. Following this, using global momentum considerations, the Poisson brackets for the coupled system in a body-fixed frame will be presented and the relation between the two brackets discussed. Special attention will be paid to the neutrally buoyant rigid body case. Comparisons between this problem and the problem of the coupled dynamics of a rigid body and discrete singular vortices will also be made Refs. [2, 3].

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# Self-Propulsion of Mobile Robots with Underactuated Internal Dynamics

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The configuration manifold for a mobile robot generally exhibits the structure of a principal fiber bundle $\pi : Q \to B$, with distinct points in $B$ representing distinct internal configurations of the robot and each fiber diffeomorphic to a Lie subgroup of $SE(3)$ representing feasible positions and orientations of the robot in its environment. Under certain circumstances, the mechanics of such a robot may determine a principal connection in this bundle so that the robot's capacity to propel itself via cyclic changes in internal shape reflects the holonomy of the connection. The connection may manifest, for instance, a nonintegrable distribution of constraints on the robot's motion or a conservation law resulting from the invariance of the robot's kinetic energy under the lifted action of the bundle's structure group on $TQ$. This perspective is explored in [1] and elsewhere, but the supposition in the robotics literature is typically that such a robot has complete control over its internal shape, and that the problem of motion planning primarily concerns the identification of closed paths in $B$ that generate desired geometric phases.

Underactuated internal dynamics may be a design feature rather than a shortcoming for a mobile robot. Physical experiments have shown, for instance, that if the actuators at certain joints within an articulated swimming robot are replaced with springs, these joints can be excited indirectly to contribute to the propulsion of the robot just as actuators would, and that partly supplanting actuation with elastic compliance in this way can improve the energy efficiency of such a robot overall. No systematic method exists, however, for optimizing the distribution of actuation and elasticity within such a robot.

This talk will address the basic problem of generating geometric phase in the context outlined above when the dynamics on $B$ involve the interplay of actuation and damped elasticity. The objective of periodic actuation in this case is to excite a periodic elastic response so that variations in the robot's internal shape correspond to looped trajectories in $B$ that enclose nonzero net curvature. While the way in which a particular trajectory in $B$ lifts to a trajectory in $Q$ is independent of time parameterization, elasticity defines an absolute timescale, so that even a solitary actuator driven sinusoidally with respect to time can excite qualitatively distinct dynamics when driven at different frequencies. The talk will detail analyses of both terrestrial and aquatic robots, focusing in particular on an ideal-flow variation of a canonical system known as *Purcell's swimmer* [2] for which the authors have developed both computational and physical models.

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# Separation of variables on spaces of constant curvature

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The Hamilton-Jacobi equation provides a deep and powerful formulation of mechanics, whose usefulness lies in the identification of conserved quantities; separation of variables continues to be the method of choice for obtaining exact solutions, and hence extracting the first integrals of a system. However, separation of the Hamilton-Jacobi equation is not always possible. So the question we address is the following: given a pseudo-Riemannian manifold $M$, can we classify all the orthogonal coordinate systems, up to equivalence, in which the Hamilton-Jacobi equation separates?

We review the general theory due to Eisenhart, which involves classifying certain types of Killing tensors, and integrating some differential equations. We then present a more recent and completely algebraic approach using concircular tensors, which works when $M$ has constant curvature; a detailed review of the theory can be found in [1]. We also review applications of the theory to natural Hamiltonians, highlighting some interesting examples such as the charged particle orbits. We focus our attention to Riemannian and Lorentzian spaces of constant curvature, and point out the relevance of the theory to the related Schrödinger and Klein-Gordon equations.

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# SS-IM Industrial Mathematics

# A note on fuzzy multiattribute grey related analysis using DEA

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**Abstract**

**Purpose:** Wu and Olson [Wu, D. D., and Olson, D. L. (2010). Fuzzy multiattribute grey related analysis using DEA. Computers & Mathematics with Applications, 60(1), 166-174] applied data envelopment analysis (DEA) in a grey-related fuzzy methodology to derive attribute weights that are most favorable for each alternative. However, their model may not reflect the desired degree of discrimination between alternatives for unlikely weight combinations. In this paper, we propose an extended version of their model by using two sets of weights that are most favorable and least favorable for each alternative.

**Methodology:** This research has been organized to proceed along the following steps:

1. Computing the grey relational coefficients for alternatives with respect to each attribute using a fuzzy GRA methodology. Grey relational coefficients provide the required (output) data for a series of DEA models.

2. Computing the non-zero optimal weights using a DEA model which provides the minimum weight bound for the attribute weights in the best- and worst-practice DEA models.

3. Computing the grey related grades for alternatives using the best-practice DEA model bounded by non-zero weights. The attribute weights obtained from this model are the most favorable non-zero weights for alternatives.

4. Computing the grey related grades for alternatives using the worst-practice DEA model bounded by non-zero weights. The attribute weights obtained from this model are the least favorable non-zero weights for alternatives.

5. Aggregating the grey related grades obtained from the best- and worst-practice DEA models to assess the overall performance of alternatives.

**Results:** The extended model provides a more reasonable and encompassing measure of performance for alternatives in GRA. An illustrated example of a nuclear waste dump site selection is used to highlight the usefulness of the proposed "extended model".

**The theoretical contribution:** The extended version of the Wu and Olson's model improves the validity and stability of the performance measures for alternatives in a fuzzy GRA framework, without needing a *priori* information about attribute weights.

**Keywords**: Grey related analysis, Data envelopment analysis, Fuzzy numbers, Multiple attribute decision making, Weighing.

**Abstract**

Matrix factorization is one of the widely used methods of data analysis. Generalized Coupled Tensor Factorization (GCTF) framework generalizes matrix factorization to work with multiway tensor data by deriving update rules to compute latent tensor objects in tensor factorization problems. Tensor Factorization Toolbox (TFT) implements GCTF in Matlab environment. This paper introduces TFT, presents the factor graph notation we use to visualize the underlying tensor operations required by GCTF update equations and algorithms we developed to search for the optimal operation order in a single tensor operation and GCTF update rules.

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# Estimating the Crossover Point of a Fuzzy Willingness-to-Pay/Accept for Health to Support Decision Making

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Deciding which of the health technologies (HTs) offered by the industry to reimburse requires juxtaposing two very different criteria—health and money—preferably from the societal perspective, as public funds are involved. Health is a non-market good (unlike health services); hence, people's preferences may be imprecise due to lack of trading experience. Still, to make the health technology assessment (HTA) process tractable, this imprecision should be handled formally, with quantitative methods.

Jakubczyk & Kamiński (henceforth, J&K, [1]) introduced a model of preferences between HTs when willingness-to-pay/accept (WTP/WTA) are treated as fuzzy sets. J&K surveyed a sample of HTA experts in Poland (mostly from the industry or the regulator); the respondents declared conviction (with Likert scale) that a unit gain/loss in health (a quality-adjusted life year, QALY) is worth spending/saving a given amount (of PLN, 1 PLN $\approx$ 4 USD). The survey results show that WTP/WTA is indeed perceived imprecisely, also by HTA experts. The ideas how the fuzzy WTP/WTA can be used in making a choice from $> 2$ alternatives were presented in [2].

In the present study, I further develop the above ideas and argue why decisions should be based on the crossover point (CP) for fuzzy WTP/WTA (informally, a value that the respondent is equally convinced it is or is not worth paying/accepting for a QALY). As the major contribution, I show three ways to statistically infer about the CP based on random samples: (1) hypothesis testing, adapting a Dykstra test [3]; (2) hierarchical Bayesian approach; and (3) frequentist meta-analytic approach. I test these approaches on data from J&K.

We cannot reject the null hypothesis that the CP for WTP amounts to 125 or 150 (all results in 000s PLN/QALY), and for WTA—to values between 150 and 300. Bayesian modelling yields the point estimates of WTP=145.7 and WTA=162.3 with the 95% credible intervals of $(107; 197.9)$ and $(115.8; 228.1)$, respectively. The frequentist approach yields the point estimates of WTP=153.6 and WTA=163.3 with the 95% confidence intervals of $(121.2; 202.9)$ and $(120.9; 225.1)$, respectively. The estimates exceed the official threshold at the time of the survey, 119.6. The results rebut the need to account for WTP-WTA disparity in decision making, cf. [4]. On the other hand, estimating the CP results in stochastic uncertainty, that should be accounted for in the sensitivity analysis.

The methods used in the present study can be employed in other situations where a non-market good must be valued, e.g. as an input to cost-benefit analysis. Hence, the presented techniques can be implemented beyond HTA, e.g. to support the environmental decision making.

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# Fuzzy Approach to Elicitation of Preferences Towards Health States

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Health care is largely financed with public resources, and the public regulator chooses which drugs to reimburse. To make such decisions in an informed way, we need to measure and compare the effectiveness of available technologies (how much health is bought), accounting for the improvements in both the quality and the longevity of life. Typically, in this health technology assessment process, the amount of health is measured with quality-adjusted life years (QALYs), i.e. the equivalent number of years in full health; in the QALY model the utilities must be assigned to individual health states. Th preference elicitation in applied research is more and more often done by conducting discrete choice experiments (DCEs): presenting to a group of respondents a number of pairwise choice problems between two health descriptions. Then, in the standard approach, we assume that individual choices result from some true, underlying, crisp preferences (plus a stochastic error term); the underlying preferences may be estimated by econometric modelling [1].

Most people consider health (quality and duration of life) as important but since we rarely choose between health states, our preferences may not be well-formed; moreover, the quality of life in research is frequently defined using imprecise terms (e.g. *moderate* difficulties doing *usual activities*). Therefore, we propose to model preferences towards health states (precisely: disutilities of worsening health dimensions in the EQ-5D-5L descriptive system [2]) as fuzzy [3], assuming each worsening is assigned an interval (range of values), instead of a crisp number.

We elicit such preferences with DCE data, using a maximum likelihood approach and bootstrapping to assess the estimation error. We find, for example, that pain/discomfort and anxiety/depression are associated with the largest upper bounds of disutilities and the largest fuzziness (widest ranges).

Our approach dispenses with one of the non-intuitive features of the standard approach to DCE, where even a clearly dominated alternative has a positive probability of being chosen: in our model, if the disutility ranges do not overlap the worse alternative will never be chosen. Also, our model offers a more consistent approach to the constant proportional trade-off condition: the probability of a given health state being chosen in a pair will not change if durations are scaled proportionally; something that is not true in the standard DCE model. We believe that incorporating imprecision to modelling preferences towards health states also increases the face validity.

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# Mathematics of Blockchain
# A Double-Edge Sword Helping Criminals and Thwarting Fraud

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Blockchain is a distributed ledger technology, the design of which was first released publicly in 2008 through a white paper of an anonymous developer who goes by the pseudonym Satoshi Nakamoto. A blockchain ledger is a record of transactions that is shared across a network of users and individually verified by each participant. Transactions are grouped together and tied to all previous transactions using a cryptographic technique called hashing. Blocks of transactions linked together in this way make altering the record nearly impossible. The difficulty is further increased by the distributed nature of the system, which would require an alteration to be made simultaneously across all the network's participants to be successful – something that becomes more difficult as the user base grows.

Blockchain technology first became famous for its use as the primary technology enabling the Bitcoin cryptocurrency designed by Nakamoto. Until then, there had been many attempts at creating a secure and practical digital cash system, but none of them became as successful or as widespread as Bitcoin. Today, Bitcoin is used by libertarians, who wish to stay away from the mainstream banking systems due to their ideology, as well as organized criminals, who are evading law enforcement taking advantage of anonymity and intractability of Bitcoin.

Since 2009, the blockchain technology has continued to be developed for use in numerous different applications and industries. The technology has the potential to disrupt existing markets because it has solved a fundamental problem with creating a digital economy: How do you prove ownership of an asset in an environment where everything can be copied or modified? With this problem solved, the internet can be used as the foundation to build out a large-scale transaction processing platform. Blockchain can also be used to fight fraud in many industry vectors. In financial industry, for instance, blockchain can facilitate identity management and Know-Your-Client efforts.

In this talk, we look at the mathematics behind this double-edge sword. We go back as early as 1990 CRYPTO conference paper of Haber and Stornetta who proposed a data-structure for appending a series of temporally-ordered messages to each other. We discuss the hashing mechanism that secures the Bitcoin and other common Blockchain implementations. Moreover, we cover the mathematics behind the common consensus mechanisms as well.

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# Modelling Calcite Dissolution in a Rotating Disk Reaction Vessel

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The carbonate system is one of the most complex and widely present chemical systems in the nature, playing a role in many natural and industrial processes. This talk will review the underlying chemistry of this system in a controlled environment, a rotating disk reaction vessel, and compare the formulation of the problem with the traditional chemical literature. Combining the free boundary Stefan condition with the limiting conditions of the chemical environment naturally provides a boundary condition at the dissolution/precipitation interface. This condition depends on the external parameters (pressure, temperature, pH) and is traditionally given by an experimentally determined reaction rate at the surface. A comparison is made to the experimentally determined PWP (Plumber, Wigley, Parkhurst) expression that is currently used as an externally imposed constraint. This model has the advantage of reproducing the observed behaviour as an interconnected system between the dissolving surface and the bulk without the need to introduce additional reactions occurring at the reacting surface.

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# Modelling of Superparamagnetic Beads and the Optimal Placement of Cells in Deep Tissue

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Colonization of porous scaffolds with cells is of increasing importance for various tissue engineering applications. To this end, human endothelial cells (ECs) loaded with superparamagnetic beads by phagocytosis were used for seeding micro-porous, poly-caprolactone scaffolds prepared by electrospinning. This talk is broken into two separate aspects. The first half considers the beads themselves and how the manufacturing process of the beads and how the size of the beads affects their collective magnetic behaviour. The second half details the problem of scaffold colonization whereby collections of cells with varying numbers of embedded beads are placed at predetermined locations within the scaffold with some form of control.

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# Towards Imaging Molecules from Coulomb Explosions

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In the last few years a new rapid imaging technology has provided the capability to view molecular reactions as they are taking place. Pixel Imaging Mass Spectrometry [1] relies on precision laser pulses to both align and strip molecules of their valence electrons causing them to suffer a Coulomb explosion. The holy grail of this technology is to find an efficient algorithm to determine the structure of the parent molecules by systematically collecting the resulting explosion fragments. This talk will dices the aspects of the forward problem for the highly structured parent molecule parent molecule 3,5-dibromo-3',5'-difluoro-4'-cyanobiphenyl. In particular, the predicted time-of-flight (TOF) spectra will be compared to the experimentally obtained result. Aspects of the inverse problem (determining the parent structure from the observed spectrum and covariance maps) will also be discussed and some preliminary results presented. For larger molecules, where this experimental technique is expected to be superior, the TOF spectrum becomes congested necessitating the development of alternative strategies to resolve the structure of the parent molecule.

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# SS-MFMCR Mathematical Finance — Modeling, Computation and Risk Management

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# A geometric approach to arbitrage-free modelling, estimation, and prediction

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We develop a new approach to stochastic modelling, estimation, and prediction in mathematical and computational finance. In the modelling step, we show how to obtain an optimal model by exploiting the implicit geometry characterizing the class of arbitrage-free models. Since the resulting optimal model is non-Euclidean, estimation and implementation is performed using new manifold learning algorithms. We conclude by showing these models best balance the nonlinearities and financial information present in the data. Moreover, the manifold learning algorithms have greater predictive power than their classical Euclidean counterparts.

# A New Risk-based Approach for Pricing High-Dimensional American Options

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**Abstract.**

Pricing American high dimensional option is one of the essential problems in computational finance. Many researchers in the financial markets truly believe that mispricing or incorrect valuation of these securities would be the main reason of collapse in some financial organizations. The complexity of option pricing, especially in the case of American basket options, which are a type of high dimensional options, has motivated many researchers to develop numerical and simulation-based models for pricing options. In this paper, a new simulation-based approach for pricing of American basket option with consideration of risk is proposed. Having the prices obtained through Longstaff-Schwartz methodology, which is based on Approximate Dynamic Programming (ADP) as a risk-neutral approach, we extend lower and upper bounds for the price of the American basket option according to worst-case (pessimistic/risk-averse) and best-case (optimistic/risk-taking) scenarios. Furthermore, for scenarios generation, we use a Monte Carlo simulation technique using a t-student copula-GARCH method and Extreme Value Theory to handle the nonlinearity of dependencies between variables. To verify the computational efficiency and the accuracy of the proposed methodology, we compare the results of prices obtained through these proposed models with those ones achieved from the Monte Carlo method for European basket options. Moreover, the developed models are tested using out-sample scenarios to explore what would happen if the investors bought the option with the obtained prices through three different strategies: risk-averse, risk-neutral, and risk-taking approaches.

**Keywords:** American Basket Option Pricing, Approximate Dynamic Programming, Risk-based Pricing, Monte Carlo Simulation.

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# Bankruptcy Prediction and Default Detection Using Genetic Algorithm-Support Vector Machine and Information Complexity

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Bankruptcy and defaulting at the individual and company level has become a prelevant incident in industrial countries during economic crisis. For example, we have a consumer credit system in which the risk of an individual, company, or even system collapse rises with every increase in debt. There is indeed "a clear and pressing need for interdisciplinary research and education aimed at addressing the stream of corporate scandals that continues to roil the global economy." (cf. RFP-2-26-09).
A common problem in all clustering techniques is the difficulty in choosing the number of clusters or patterns present in a given data set with defaulting and non-defaulting companies; determining which variables that will best predict between the clusters chosen; and identifying the defaulting companies at the micro level.
A current benchmark data set on bankruptcy and defaulting will be used that will include the financial characteristics of over 1000 companies on high dimensional explanatory variables on several categories such as: Liquidity Ratios; Activity Ratios; Profitability Ratios; etc; to mention a few to develop, train, and validate the proposed techniques for bankruptcy prediction and default detection.

Namely this paper shows that Genetic Algorithm (GA)-Support Vector Machine (SVM) approach outperforms other statistical pattern algorithms for bankruptcy prediction and default detection using information complexity criterion and genetic algorithms.
Along with this advancement, specialized variants of the (GA-optimization heuristics) will be hybridized to determine the best subsets of bankruptcy predictors by using a novel statistical modeling and model selection procedures based on information complexity criterion(ICOMP) criterion of Bozdogan (1988, 1990, 1994, 2000,...) as our fitness function to improve the computational time.

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# Abstract

In this paper, co-movements between gold price, Rial to Dollar exchange rate, Tehran stock index, and OPEC oil price time series are examined using Continuous Wavelet Transform. Two main advantages of Wavelet Transform against other approaches are: 1) investigating the time series in the time and frequency spaces synchronously, and 2) using functions, namely mother wavelets, which are capable of analyzing non-stationary time series.

In the following, the variances of each time series, covariances of their pairs, and co-movements of them have been determined in every single point of time-frequency plane, using Wavelet Power Spectrum, Cross Wavelet Spectrum, and Wavelet Coherence Spectrum, respectively. Subsequently, the noteworthy results show that Gold can be the proper hedge against Rial depreciation in the long term, while in the short term, it can play the safe haven role for exchange rate fluctuation. Finally, by using phase differences of Wavelet Coherency, the time leads/lags have been calculated by which the investors and policy makers are able to make proper decisions.



**Key Words:** Co-movements, continuous wavelet, cross wavelet, wavelet coherency, gold price, exchange rate, oil price, stock index, Iran

# Hedge funds: will we see negative management fees?

Luis Seco

May 5, 2017

**Abstract**

Low negative rates and small performance environment are putting pressure on the hedge fund business. In this talk we will analyze the valuations of fee structures, and propose frameworks where the Black-Scholes valuation of new fee structures delivers value to managers and investors alike.

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# Longevity bond pricing in equilibrium

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We consider a partial equilibrium model for pricing a longevity linked bond in a model with stochastic mortality intensity that affects the income of economic agents. The agents trade in a risky financial security and in the longevity linked bond in order to maximize their utilities. Agent's risk preferences are of monetary type and are described by BSDEs (backward stochastic differential equations). The endogeneous equilibrium bond price is characterized by a BSDE. By using Clark-Haussmann formula, we prove that our longevity bond completes the market. Numerical experiments present the prices of two types of longevity bonds.

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Monte Carlo Simulation in Counterparty Credit Risk

Karl Wouterloot

Monte Carlo simulation is a fundamental tool underlying Counterparty Credit Risk (CCR) measurement. CCR simulation is used for risk management applications in the computation of potential future exposure and regulatory capital. Also, it is used by the front office for XVAs in the pricing of over the counter derivatives. Computationally, CCR simulation is very complex, as typically requires the simulation of prices of portfolios with thousands of trades. Also, the choices of simulation modelling frameworks which are well-suited for the computational demands of CCR simulation are limited. This talk explores some of the theoretical and computational challenges faced in the CCR industry today, as well of some of the important innovations in the field.

**Optimal Hedging of Nontradable Risk in Discrete Time Financial Market Models**

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We consider the problem of optimal static and semi-static hedging of nontradable sources of risk. Under general model assumptions, we find a representation of an optimal hedging option on a traded security that can be used to mitigate the overall risk of a portfolio. As the criterion of optimality we use the expectation of the shortfall weighted by some loss function. Because of the use of asymmetric risk measures, the resulting hedging methods guard better against large losses when compared with more traditional approaches based on a quadratic criterion.

The representation of the optimal strategy that we obtain is amenable to implementation under a wide range of assumptions about the model. We illustrate our framework by applying it first to the problem of optimal hedging of path-dependent options, and then to the problem of optimal hedging for a risk-averse producer of agricultural commodities under different sources of risk, including price, basis and yield uncertainty. For the first application, we demonstrate that different classes of path-dependent options give rise to different rates of convergence of the residual risk when hedging using only European options. In the second problem, we explain how our framework can be used to study implications of different assumptions about the copula function that determines the dependence structure of the involved risk factors.

# PRICING AND HEDGING DERIVATIVES ON DIVIDENDS

NICK COSTANZINO AND TAI-HO WANG

Dividends are notoriously difficult to model and often lead to inconsistent financial and economic theories. This is embodied no more so than in the *Dividend Puzzle* first described by Fischer Black whereby under the Modigliani-Miller theory the dividend policy of a firm should have no bearing on the price of equity even though empirical results show otherwise. One of the difficulties is that, traditionally, dividend exposure has been intertwined with equity exposure through swaps and other such products. Recently, exchange traded derivatives on dividends have appeared on several indices such at the S&P500 on CBOE, EUROSTOXX50 on EUREX and Nikkei225 on JPX. These products allow investors to express a cleaner and more direct view of dividends and establish dividends as a separate asset class. In addition, these new products allow for the better modelling of dividends and their relationship to equity.

In this talk we propose a general framework to price derivative contracts on dividends when the underlying follows local volatility dynamics and the dividend is modeled as an arbitrary function of the underlying. We then discuss calibration and hedging strategies and their relation to Dupire's equation.

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# Robust multivariate portfolio choice with stochastic covariance in presence of ambiguity

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In this talk, we provide the optimal multivariate intertemporal portfolio in closed form for an ambiguity averse investor, who has access to stocks and derivative markets.
The stock prices follow a stochastic covariance process and the investor can have different levels of uncertainty about the diffusion parts of the stocks and the covariance structure. The alternative model for the stock, eigenvalues and option prices reads:

$$\begin{aligned} dS_t &= D[S_t]\left(r + AV_t^{\frac{1}{2}}(\lambda_t^S - e_t^S)\right)dt + D[S_t]AV_t^{\frac{1}{2}}d\tilde{W}_t^S \\ dv_t &= \left(K(\bar{v}-v_t) - \Sigma_t^v\left(Re_t^S + (I-R^2)^{\frac{1}{2}}e_t^v\right)\right)dt + \Sigma_t^v\left(Rd\tilde{W}_t^S + (I-R^2)^{\frac{1}{2}}d\tilde{W}_t^v\right) \\ dO_t &= D[O_t]\Big[\Big(r + PV_t^{\frac{1}{2}}(\lambda_t^S - e_t^S) + QV_t^{\frac{1}{2}}(\lambda_t^v - e_t^v)\Big)dt + PV_t^{\frac{1}{2}}d\tilde{W}_t^S + QV_t^{\frac{1}{2}}d\tilde{W}_t^v\Big], \end{aligned}$$

We find strong evidence that the optimal exposures to stock and covariance risks are significantly affected by ambiguity aversion. Welfare analyses show that in both, complete and incomplete markets, investors who ignore model uncertainty incur large losses, larger than those suffered under the embedded one-dimensional cases. We further confirm large welfare losses from not trading in derivatives as well as ignoring intertemporal hedging.

This work studies the setting of [Escobar et al. 2015] in multidimensions while assuming model mis-specification in [Escobar et al. 2016].

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# Simulation of Multivariate Mixed Poisson Processes

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Multivariate mixed Poisson processes have many important applications in Insurance, Finance, and many other areas of Applied Probability. In this paper, we extend the Backward Simulation (BS) approach [1] to modelling multivariate mixed Poisson processes and analyze the connection to the extreme measures describing the joint distribution of the processes at the end of the time horizon. The BS approach relies on the conditional uniformity of the arrival times, given the number of events and allows for the correlation coefficient between Poisson processes to take extreme values. In an earlier work [2], the forward continuation of the BS was introduced for Poisson processes in order to achieve richer correlation profiles. It was also shown that the forward continuation of the BS is asymptotically stationary. Along with the extension of the BS to multivariate mixed Poisson processes, we investigate the forward contiunation of the BS approach for multivariate mixed Poisson processes.

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# SS-MMNN Mathematical Models for Nanoscience and Nanotechnology

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# Longitudinal and Transverse Plasmon excitations in Electron Energy Loss Spectroscopy of Graphene

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Strong interaction between light and quasi-free electrons in matter gives rise to Plasmonics as a separate branch of Nano-photonics, which enables one to break the diffraction limit and concentrate light into deep-subwavelength volumes with huge field enhancements. As the use of graphene is rapidly growing, new scientific and technological opportunities are opened in the context of Optoelectronics and Photonics. Highly doped graphene is considered to be a promising plasmonic material working in the mid-infrared and terahertz spectral ranges.

Excitation of surface plasmons by swift electrons has long been utilized in electron microscopes for experimental technique called electron-energy-loss spectroscopy (EELS) to investigate plasmonic properties of ultrathin, or two-dimensional electron systems. In electron microscopes it is possible to focus electron beams on subnanometer spots and probe the target response by analyzing electron energy losses or by detecting emitted radiation. The theoretical investigation of energy losses and transition radiation (TR) resulting from the elastic interaction of fast charged particles traversing graphene sheets has quite amazing results and is very productive research nowadays.

When a single graphene sheet is probed by a normal fast charged particle in retarded regime, one can expect the excitation of a single longitudinal plasmon mode and symmetric TR [1]. Probing the multi-layer graphene structure, however, enables us to have asymmetric longitudinal plasmon modes excitations and asymmetric TR. These plasmons have very high tunability due to the change of the velocity of the particle and the inter-graphene distance [2].

One, also, may excite the transverse plasmon in a single graphene sheet. This may be happening by an angled probing charged particle traversing the graphene sheet. However, analysis of the dispersion relation for the transverse plasmon i.e.

$$\lambda_t = 1 - i\omega\frac{2\pi}{qc^2}\sigma = 0, \tag{1}$$

shows that one should take the interband transitions in graphene conductivity into account to produce real mode.

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# Modeling the Interactions of Graphene with a Liquid Electrolyte

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Graphene has found applications in electronics and photonics, but in recent years, a new application of graphene based materials for bio-sensing has materialized [1, 2, 3]. Typically, graphene-based sensors function as a field effect transistor (FET) where graphene is in contact with a liquid electrolyte [4, 5]. These transistors can be used as biological and chemical sensors, with sensitivity to pH and ion concentration arising from the adsorption of ions to the graphene-electrolyte interface, and typically operate under high ion concentration and high surface charge density [6, 7]. This regime complicates mathematical modeling based on the Poisson-Boltzmann (PB) equation as dielectric saturation and ion crowding become non-negligible at the interface.

While there is plenty of experimental work done in the sensing applications of electrolytically gated graphene FETs, the theoretical modeling lags significantly behind experiments, which is unlike other areas of applications for graphene and may be partially due to the interdisciplinary nature of the problem. In recent years, there has been some success with modeling the capacitance of graphene-based FETs under equilibrium conditions and on the screening mechanisms due to mobile ions in the electrolyte, which were accommodated through modifications of the PB equation [4, 5, 8]. It still remains to develop a full model which accurately predicts experimental results.

In this work, we showcase the interplay between the ion steric effects and the dielectric saturation in solvent, expose the importance of quantum capacitance when graphene is used as an electrode, and demonstrate the importance of the Stern layer in continuum models of the electrode-electrolyte interface [9]. We will also highlight how the ion polarization in the solvent affects capacitance of the diffuse layer and the overall system's capacitance.

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# Modelling and design of nano-structures: multilayer nanoplasmonics configurations

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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 [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 would 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 at sub-wavelength dimension. In 1899, Sommerfeld had described surface waves (waves propagating at the surface of metals) mathematically, and in 1902 Wood observed anomalous drops in the intensity of light reflected by a metallic grating [2]. But theory and observation would not be linked until 1941, by Fano [4]. Further experimental validation came in 1968, when Kretschmann and Raether used prism coupling to excite surface waves with visible light [5]. Other forms of coupling to surface plasmons have been thoroughly investigated since then. All of the phenomena mentioned above are based entirely on classical electromagnetics, and thus can be mathematically described by Maxwell's equations. In this talk, an integral-equations formulation is given for multilayered an infinitely periodic metal configuration whose period $d$ is on the nanometer scale. This configuration is composed of a thin layer of metal with depth larger than skin depth of the material, buried into different epoxies on top (glass/polymer substrate) and the bottom (liquid/water/blood) both extend infinitely above and below the surface. Some details of the numerical implementation and the preliminary results of a few numerical experiments will be given in this talk.

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# Nonlinear Coupled Effects in Nanomaterials and their Application for Energy Harvesting

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The behaviour of materials at the nanoscale is characterized by quantum effects which influence their properties. For example, some nanomaterials have the ability to convert between mechanical and electrical energy due to the presence of electromechanical coupling in the material. This phenomenon known as the piezoelectric effect has been used in the form of nanogenerators to harvest clean and renewable energy from abundant mechanical energy sources in the environrment. Energy harvesting using nanogenerators involves inducing mechanical strain in nanomaterials to discharge current or voltage. Electrical energy created in this manner does not have environmental limitations. Recent experimental results have shown that accounting for the nonlinear piezoelectric effect in nanomaterials produces outcomes significantly different from those obtained by using conventional linear models [1], [2]. The goal of this research is to examine, using techniques of mathematical modelling, the effects of nonlinear piezoelectric effect on the time-dependent, coupled thermo-electro-mechanical (TEM) interactions inside the nanomaterial, and its contribution to applications of nanomaterials for mechanical energy harvesting. The time-varying TEM behaviour is modelled using the classical continuum approach that has been known to successfully predict the behaviour of nanodevices [3]. The mathematical model that is constructed to account for the coupling between thermal, electrical, and mechanical fields is based on the Fourier, Poisson, current continuity, and elasticity equations. The system of PDEs thus obtained is solved numerically using the finite element method. It has been known that the time-dependent temperature variation in some nanomaterials coupled with their semiconducting properties, successfully generate electric polarization and charge separation in low dimensional nanostructures fabricated using these materials. Therefore, by introducing time dependence in the TEM coupled system we observe further enhancement of the charge separation inside the nanomaterial, which increases current flow in the nanogenerator. In addition, accounting for the decay of excess charge carriers over time in the current continuity equation is expected to give a more realistic model of current generation inside the nanogenerator. This novel time-dependent TEM system and its numerical analysis is the main focus in this contribution.

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# Nonlocal optical response of nanowire-film system: gap effects

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In this paper, we present a computational analysis of the electromagnetic response of a nanowire-film system. The computed solution accounts for the non-local response of the plasmonic media (vacuum). The system under consideration consists of a nanowire made of a noble metal such as gold (Au) placed over a film of the same material. Such a nanostructure exhibits an optical response that is extremely sensitive to the gap between the nanowire and film which makes it favorable for various sensing applications. The non-locality of the plasmonic medium, which can be captured with the hydrodynamic model, significantly affects the resonant wavelength ($\Delta\lambda_{res}$) of this system for structures of small dimensions (less than 5 nm gap between the nanowire and the film). We present new computational results that can be used to predict the effect of non-locality on the resonances of the system.

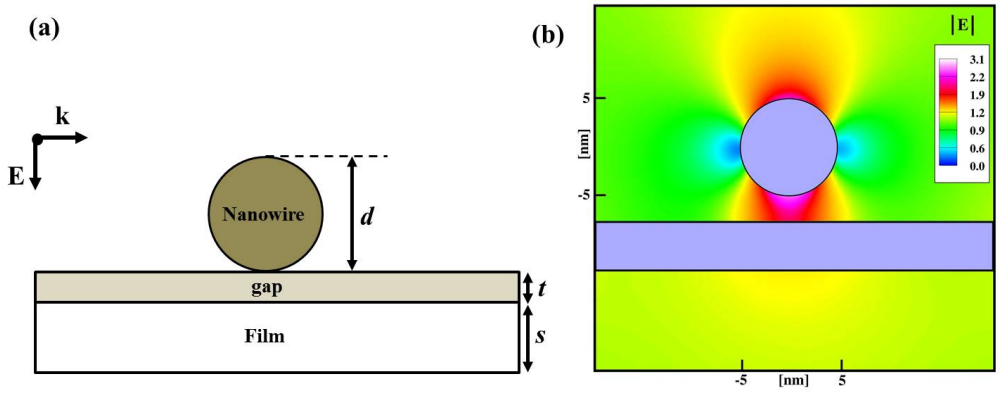


Figure 1: (a) Schematic diagram of nanowire-film system, (b) normalised field profile $\left(|E|\right)$.

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# Photoluminescence in Quantum Emitter and Metallic Nanoshell Hybrids

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Recently, there has been considerable interest in the study of metallic nanoshells (MNSs) for the application of nanomedicine. MNSs are generally fabricated by coating a spherical dielectric nanoparticle with a metallic shell. Surface plasmon polaritons (SPPs) are present at the interface between the core dielectric material and the metal. The wavelength of the surface plasmon polaritons and the absorption efficiencies in nanoshells can be controlled through the size and composition of each layer of the nanoshell structure. These structures have attracted significant interest because they are a novel platform for nano-biotechnology and nanomedicine due to their convenient surface bio-conjugation with molecular probes. They are also an important building block of nano-medicine due to the desirable SPP resonances. Metallic nanoshells have been fabricated by many groups to study their optical properties for applications in nanomedicine. They have also been used in cancer therapies [1,2] due to their absorbing properties. In this work, we have studied the photoluminescence emission in a quantum emitter (QE) and metallic nanoshell (MNS) hybrid system. Surface Plasmon polariton resonances in the MNS are calculated using Maxwell's equations in the quasi-static approximation. It is found that the MNS has two SPP resonances. We have also compared our theory with the extinction coefficient of MNSs made up of gold shell and silica core. A good agreement between theory and experiment is found. A probe laser field is applied to study the photoluminescence (PL) spectrum in the hybrid system. Dipoles are induced in the MNS and QE due to the probe laser. Hence the QE and MNS interact via the dipole-dipole interaction. The PL spectrum of the QE is calculated using the density matrix method in the presence of the dipole-dipole interaction. It is found that the PL spectrum of the QE with degenerate excitons splits from one peak to two or three peaks depending on the locations of two SPP resonances. Similarly, for the nondegenerate QE we found that the PL spectrum splits from two peaks to four peaks. These interesting findings can be useful in the fabrication of nanosensors, nanoswitches and for other applications in medicine.

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# SS-MSED Modeling of Socio-Economic Dynamics

# An age-structured continuum model for myxobacteria

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**Abstract**

Myxobacteria are social bacteria, that can glide in 2D and form counter-propagating, interacting waves. Here we present a novel age-structured, continuous macroscopic model for the movement of myxobacteria. The derivation is based on microscopic interaction rules that can be formulated as a particle-based model and set within the SOH (Self-Organized Hydrodynamics) framework. The strength of this combined approach is that microscopic knowledge or data can be incorporated easily into the particle model, whilst the continuous model allows for easy numerical analysis of the different effects. This allows to analyze the influence of a refractory (insensitivity) period following a reversal of movement. Our analysis reveals that the refractory period is not necessary for wave formation, but essential to wave synchronization, indicating separate molecular mechanisms.

**Key words:** Self-propelled particles, nematic alignment, hydrodynamic limit, generalized collision invariant, diffusion correction, myxobacteria, wave formation, refractory period.

**AMS Subject classification:** 35L60, 35K55, 35Q70, 82C05, 82C22, 82C70, 92D50

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# Inhomogeneous Boltzmann-Type Equations Modelling Opinion Leadership and Political Segregation

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In this talk we present a kinetic model for modelling opinion dynamics. Such models successfully use mathematical tools from statistical mechanics to describe the behaviour of a large number of interacting individuals in a society. This leads to generalizations of the classical Boltzmann equation for gas dynamics. Most approaches in the literature assume a homogeneous society. To allow for additional sociologic effects that play an important role in real societies, e.g. the influence of opinion leaders, we discuss their extension to an inhomogeneous setting.

We present kinetic models for opinion formation in which the opinion dynamics depend on an additional independent variable, e.g. a leadership or a spatial variable. More specifically, we consider: (i) opinion dynamics under the effect of opinion leadership, where each individual is characterised not only by its opinion, but also by another independent variable which quantifies leadership qualities; (ii) opinion dynamics modelling political segregation in 'The Big Sort', a phenomenon that US citizens increasingly prefer to live in neighbourhoods with politically like-minded individuals. Based on microscopic opinion consensus dynamics such models lead to inhomogeneous Boltzmann-type equations for the opinion distribution. We derive macroscopic Fokker-Planck-type equations in a quasi-invariant opinion limit and present results of numerical experiments.

Based on joint work with M.-T. Wolfram [1].

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# Kinetic Models of Conservative Economies with Welfare Thresholds

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Kinetic exchange models of markets have been used to recover and analyze characteristics of wealth distributions using tools from econophysics. The standard treatment is to consider microscopic binary interactions where the fractional amounts of individuals' wealths that are transferred in a trade are determined by random variables; a corresponding Boltzmann equation then describes the evolution of the macroscopic wealth distribution [1]. We develop a kinetic model of wealth redistribution that - instead of consisting of transfers of random fractional amounts of wealth - deterministically aims to bring individuals with wealth below a fixed welfare threshold up to it.

This model uses need-based transfers where welfare occurs via binary gifts from individuals above threshold to individuals below [2], both randomly chosen. Using appropriate probability distributions we design policies that lead to preferential choosing of donors based on wealth corresponding to *regressive*, *progressive*, and *flat* policies. We find that the regressive policy has a higher rate of convergence, thus a faster rate of lifting individuals out of poverty. It also results in fewer individuals below threshold in steady state. However, it also leads to a wealth distribution with greater inequality. In contrast, a progressive policy leads to a higher number of individuals below the threshold but a wealth distribution with a much smaller Gini index (less inequality). The kinetic model confirms similar results based on agent-based simulations [3].

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# Mean-field control hierarchy in consensus modelling

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In this talk I will present some recent developments on a class of numerical methods for the optimal control in consensus modeling, where main goal is to steer a multi-agent systems towards a desired state. From the mathematical view point, due to the high-dimensionality and non-linearities of this type of problems, direct approaches usually inefficient. In order to reduce the high-complexity of the problem, we propose an alternative framework based on the approximation of the microscopic dynamics through Boltzmann equation, showing that under a suitable scaling this is equivalent to the mean-field description of the original optimal control problem. Thereafter, I will present a class of algorithms, based on the simulation of the binary interactions of the Boltzmann dynamics, which allows to solve efficiently the mean-field optimal control problem. Several numerical example will show the effectiveness of the proposed strategies, in the context of opinion formation and crowd motion applications.

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# Statistical Equilibria in a Discrete Choice Model of Financial Markets

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The aim of this paper is (i) to propose a discrete-choice model to study properties of statistical equilibria in a financial market, and (ii) to elucidate the causes of speculative bubbles and the crashes that inevitably follow. We consider an asset market in which risky assets and risk-free assets are traded. Investors are divided into two groups—fundamentalists and noise traders—having different decision-making rationales. Fundamentalists maximise the expected utility of their wealth in the period following their rational assessment of the fundamental value of a risky asset. Noise traders maximise the random utility of a binary choice [1]: buying bubble assets and holding risk-free assets. The noise trader's behaviour is modelled according to the theory of discrete choice with social interaction [2], which can be considered a model of Keynes's beauty contest metaphor. We demonstrate the equivalence of the random utility model and entropy maximisation principle using conjugate theory [3]. We also demonstrate that (i) if the noise trader's psychological fluctuation (corresponding to temperature under the maximum entropy principle) is large, then the market price converges to the fundamental price, so that the efficient market hypothesis holds; however, (ii) if the noise trader's psychological fluctuation is small, then the market generates multiple equilibria, and the herd behaviour of the noise traders gives rise to a bubble, which is prolonged by their positive-feedback trading but inevitably ends with a crash, which is the first-order phase transition in the asset market. We also describe how cycles of bubbles and crashes are repeated [4, 5].

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# Stylised models for the distribution of wealth

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I present a general framework to deal with distributional problems in Economics using random exchange models. The framework makes use of random partitions of stocks and fragmentation-coagulation processes acting on these partitions. Starting from finitary versions of these models, I show how they naturally lead to continuous versions.

This is joint work with Nicos Georgiou and Bertram Düring [1].

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# Macroeconomic modelling with heterogeneous agents: the master equation approach

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We propose a mean-field approximation to a stock-flow consistent agent-based macroeconomic model with heterogeneous firms and households. Depending on their investment elasticity to past profits, firms can be either aggressive or conservative. Conversely, households are divided into investor and non-investor groups, depending on whether or not they invest a portion of their wealth in the stock market. Both firms and households dynamically change their type according to transition probabili- ties specified exogenously. The mean-field approximation consists of homogenizing the balance-sheet variables for agents (firms or households) of the same type and compute the time evolution of the corresponding average as a combination of the determinis- tic dynamic, derived from investment and consumption decisions before a change of type, and the probabilistic change in type, with an appropriate rebalancing to take stock-flow consistency into account. The last step of the approximation consists in replacing the underlying Markov chain with a continuous-time diffusive limit. We present numerical experiments showing the accuracy of the approximation and the sensitivity of the model with respect to several discretionary parameters. We then use the model to investigate the relationship between stock markets with low returns and high volatility and the proportion of firms with fragile financial positions.

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# SS-NDSA Nonlinear Dynamical Systems and Applications

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# Analytical solutions of the higher-order approximation periods for the nonlinear oscillator

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In the present paper, an analytical technique of obtaining higher-order approximation periods for the nonlinear oscillator with the square of the angular frequency depends quadratically on the velocity has been developed, which is based on the harmonic balance method (HBM). Analytical investigation of the appeared set of nonlinear algebraic equations is usually cumbersome, which is addressed by the developed technique in a novel way. In this study, the developed technique provides desired results without much numerical complexity. Moreover, a suitable truncation formula is initiated in which the approximate period measures a much better result than existing periods. The developed technique is applied to benchmark nonlinear oscillator problem with the square of the angular frequency depends quadratically on the velocity to illustrate its novelty, reliability and wider applicability. It is highly remarkable that using the developed technique a third-order approximate period gives an excellent agreement with the exact ones.

In this study, the third-order approximation has been obtained by a new technique based on energy balance method (HBM) for nonlinear oscillator $\ddot{x}+(1+\dot{x}^2)x=0$ (1)

Applying the HBM, the third-order approximate angular frequency using the truncation principle is obtained as follow:

$$\omega=\left(1+\frac{a_0^2}{8}+\frac{3a_0^4}{256}+\frac{a_0^6}{6144}-\frac{53a_0^8}{2359296}-\frac{263a_0^{10}}{56623104}+\cdots\right), \quad (2)$$

and the corresponding third-order approximate period of eq. (8) is

$$T_3^{truc}=2\pi\left(1-\frac{a_0^2}{8}+\frac{a_0^4}{256}+\frac{5a_0^6}{6144}-\frac{27.4a_0^8}{262144}+\cdots\right). \quad (3)$$

To illustrate the accuracy of obtained results, we compare with the exact period $T_{ex}$ which is stated in [2].

The second- and third-order approximate periods were obtained in this study by applying truncation principle and without truncation technique to the nonlinear oscillator defined in Eq. (1) It is highly remarkable that, using truncation principle the third-order approximate period gives almost same with exact period up to eight terms. The advantages of this technique include its simplicity and computational efficiency, and the ability to objectively find better agreement in third-order approximate period using truncation principle.

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# Asynchronous control of switched nonlinear time-delay systems via the T-S fuzzy model

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This paper studies the problem of asynchronous control of switched nonlinear time-delay systems. The asynchronous control means that the switchings between the candidate controllers and system models are asynchronous. The Takagi and Sugeno (T-S) fuzzy model is employed to approximate the subnonlinear dynamic systems. By using the piecewise Lyapunov function and average dwell time approach, the asynchronously switched stabilizing control problem for nonlinear time-delay systems is solved, which allows us to have stable and unstable subnonlinear system. Based on the derived result, the desirable controller is given. Illustrative examples are provided to show the effectiveness of the results.

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# Characterization of Fluid Dynamics in Capillary Vessels: Applications for Drug Delivery

**S.C. Abou**

**Abstract:** Delivery of sufficient dose of pharmaceutical composite in microvessels as to safely achieve its desired therapeutic care and quality of life poses severe risks. Yet, no theory is sufficiently deepened to adequately describe all of the observed viscoelastic phenomena in a variety of fluid flow conditions. In this study, pharmaceutical composite flow compatible to blood flow dynamics in capillary is explored by mapping the localization of non-Newtonian fluid as directly in live cells.

At isobaric-isothermal fluid conditions, the flow descriptors are elaborated to acquire constitutive equation and analytically solve in safe manner capillary fluid flow problems. We characterized the pathway, mechanism, and energetics associated with such conduction states, and performed the characterization of non-Newtonian rheology effects due to the plasma-rich zone that forms near the wall in capillaries. The model developed portrayed blood flow descriptors at the mesoscopic level and enabled computational framework at microvessels levels for realistic predictions of blood flow under both the normal and the pathological conditions.

**Keywords:** *Microsystems, Non-Newtonian, Rheology, Modeling and Simulation*

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# Experimental Investigation of Automatic Ball Balancer Effect On Unbalanced Rotor Vibration

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Rotor vibration due to unbalance causes a lot of problems during operation. One of the simplest ways to reduce rotor vibration is the passive balancing. Unbalanced vertical rotor is modeled by a two degrees of freedom system considering Jeffcott model assumption. A (2+n) degrees of freedom mathematical model is derived with respect to a Cartesian co-ordinate system for the unbalanced rotor with the automatic ball balancer. The model equations are expressed as state equations then solved numerically. Experimental rig is developed with a data acquisition system to enable measuring the rotor vibration amplitudes. A four balls automatic balancer is designed, manufactured, and attached to the rotor. The numerical solutions of rotor vibration with and without the balancer are obtained, and compared to the measured data to validate the mathematical model. The practical effect of the automatic ball balancer on vibration amplitudes is represented at different speed ranges.

**Keywords:** Rotor vibrations, unbalance, Online balancing, Passive balancing, Automatic ball balancer, Dynamic balancer.

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# Exponential Stability of Discrete-Time Impulsive Switched Singular Systems with Time-Delay

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In this work, we consider the discrete-time impulsive switching singular system with time-delay of the form

$$\begin{aligned} E_{\sigma(n)}x(n+1) &= A_{\sigma(n)}x(n) + f_{\sigma(n)}(n,x(n-d)), && n_{k-1}^{+} \le n < n_k \\ \triangle x(n) &= B_k x(n), && n = n_k, \quad k \in \mathbb{N} \\ x_{n_0} &= \phi, \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^N$, $n_0 \in \mathbb{Z}^+$, $f_{\sigma(n)}(n,x(n-d)) : \mathbb{Z}^+ \times \mathbb{R}^N \to \mathbb{R}^N$, $\phi \in C$ and $x_{n_0} \in C$ is defined by $x_{n_0}(s) = x(n_0+s)$ for any $s \in \mathbb{N}_{-d}$ with $d \in \mathbb{N}$ representing the delay in system (1). $A_{\sigma(n)}, B_k, E_{\sigma(n)} \in \mathbb{R}^{N\times N}$ are system coefficient matrices where $E_{\sigma(n)}$ being singular with $\text{rank}(E_{\sigma(n)}) = r < N$ and $\|E_{\sigma(n)}\| \ge 1$, the matrix pairs $(E_{\sigma(n)}, A_{\sigma(n)})$ being regular, and $B_k$ being constant matrices. $\sigma(n) : \mathbb{N} \to \mathscr{S}$ is a switching rule taking values $\sigma(n) = i$ in a finite compact set $\mathscr{S} = \{1,2,\ldots,M\}$ for some $M \in \mathbb{N}$. $\{n_k\}_{k=0}^{\infty}$ are the impulsive times that form an increasing sequence satisfying $n_{k-1} < n_k$ and $\lim_{k\to\infty} n_k = \infty$. $\Delta x(n_k) = x(n_k^+) - x(n_k)$ where $x(n_k^+)$ is the state just after the impulsive action and $x_{n_k^+}(s) = x(n_k^+ + s)$ for $s \in \mathbb{N}_{-d}$, $k \in \mathbb{N}$.

This study addresses the exponential stability problem for the above system where the impulsive effects occur as a result of switching among the subsystems. Some sufficient conditions on the exponential stability of the system are established. Firstly, we consider the system consists of stable subsystems. Secondly, exponential stability of the system consisting of both stable and unstable subsystems is considered. In both cases, the stability conditions are investigated by using the multiple Lyapunov functions along with the average dwell time switching signal and by resorting the Halanay lemma.

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## Function matrix projective synchronization between two different complex networks via hybrid control

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**Abstract**

This paper studies the issue of function matrix projiective synchronization (FMPS) for two different coupled complex networks with nonidentical nodes of different dimensions, in which the internal time delay is different from the coupling delay. Based on Lyapunov stability theory, a hybrid feedback control protocol is proposed to achieve the FMPS. The symmetric or diffusive conditions for the coupling matrices are not needed. Numerical examples are presented to illustrate the effectiveness of the theoretical results.

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# Intermittent Sampled-Data Control of Cellular Neural Networks

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Cellular neural networks (CNNs) have been investigated extensively due to their wide applications in image processing, and pattern recognition [1]. Recently, many stability criteria of CNNs have been reported, and a wide variety of feedback controllers have been designed accordingly to stabilize the CNNs.

In this talk, we will discuss the stabilization problem of CNNs. A novel intermittent sampled-data (ISD) controller will be proposed, and the ISD control mechanism will be explained. Based on a Razumikhin-type stability result in [2] and Lyapunov function method, sufficient conditions will be established to guarantee the designed ISD controller stabilize the unstable CNNs. It will be shown that the CNNs can be successfully stabilized by intermittently implemented control signal with sampled information of the CNNs' states. Moreover, it worth noting that the ISD control strategy is also applicable to stabilization and synchronization problems of various dynamical systems, such chaotic systems, Cohen-Grossborg neural networks, Hopfield neural networks, and networked multi-agent systems.

Numerical examples will be given to illustrate the main results. Two types of simulation results will be given: periodic ISD control and aperiodic ISD control. Comparison of these simulation results and some future research potentials will also be discussed.

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# Linearization and local topological conjugacies for impulsive systems

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The celebrated Hartman-Grobman theorem for ordinary differential equations states that the phase portrait nearby a hyperbolic equilibrium point of a nonlinear system is equivalent to that of its linearization by a conjugation. One consequence of this theorem is that in most cases, local analysis of a nonlinear system is sufficient to predict its qualitative behaviour for some short period of time.

Hartman and Grobman's theorem has been extended in numerous ways to accomodate more general classes of dynamical systems. For instance, generalizations have been proven for finite-dimensional nonautonomous systems, impulsive systems, and impulsive differential equations in Banach spaces [1, 2, 3]. All of the aforementioned generalized results, however, require global Lipschitz assumptions on the vector field and jump map, as well as intimate knowledge of the dichotomy properties of the linearized system. Such global conditions are present in seemingly all published linearizaton theorems for impulsive systems. Since many systems encountered in applied fields are nonlinear and not globally Lipschitz, there is a need to weaken the assumptions. In this talk, we show that one can localize these linearization theorems near a hyperbolic equilibrium point, provided sufficient smoothness conditions are satisfied and time-varying terms are suitably bounded. Global assumptions on the nonlinearity are no longer necessary and one does not require as detailed an analysis of the linearized system to apply the result.

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# Modeling of Bubble Motion in a Viscid Liquid under Microgravity

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A nearly spherical gas bubble expands adiabatically in a viscous incompressible liquid flowing pass it. The equations of motion of the bubble are deduced using the Lagrangian procedure with a dissipation function when the bubble is projected initially vertically upwards. As the time progresses, the expanding bubble, which is projected vertically (along z- axis) with an initial velocity, is found to translate through the liquid with compulsorily progressive deformation from the spherical shape. The effect of viscosity on the deformation, velocity of the centre and radius **R** with time are investigated. The viscosity and initial deformation are found to influence the early stage of the growth of the nearly spherical bubble motion with time. It is seen that effect of initial deformation on the shape of the bubble as the time progresses is more significant than that of viscosity.

On neglecting the deviation of the bubble from its spherical shape, the motion displays a periodicity in time. The momentum of the fluid, displayed by the gas bubble in the direction of the motion of the bubble, is found to be constant in the absence of viscosity. Both these results are given physical justification.

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# Robust reliable $H_\infty$ control and input-to-state stabilization for switched systems

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In this research work, we consider the following switched control system

$$\dot{x} = (A_i + \Delta A_i)x + B_i u + G_i w + f_i(x), \qquad i \in \mathscr{S} = \{1,2,...,N\} \tag{1}$$

$$z = C_i x + F_i u, \tag{2}$$

$$x(t_0) = x_0 \tag{3}$$

where $x \in R^n$ is the system state, $A_i$ is a non-Hurwitz matrix for each $i$, $u \in R^q$ is the control input, the matrix pair $(A_i, B_i)$ is stabilizable, $w \in R^p$ is an input disturbance which is assumed to be time varying with norm-bounded energy, $z \in R^r$ is the controlled output, $f_i(x) \in R^n$ is nonlinear lumped uncertainties or perturbation, $A_i$, $B_i$, $G_i$, $C_i$ and $F_i$ are known real constant matrices, and $\Delta A_i$ is a piecewise continuous function representing parameter uncertainty with bounded norm.

This work addresses the problem of designing a robust feedback-reliable $H_\infty$ controller to achieve input-to-state (IS) stabilization for the uncertain switched systems, where the component failure occurs within the control actuators. While in most of the available literature on reliable controls, the faulty actuators are modeled as outages (i.e., zero output), in this work the output signal of these actuators are assumed be non-zero disturbance that will be augmented with the system input disturbance. The latter case is more practical because most of the control component failures occur unexpectedly.

The novelty in this work is to develop new sufficient conditions that guarantee the IS stabilization and $H_\infty$ performance of the switched system in the presence of the disturbance, state uncertainties, and nonlinear lumped perturbation not only when all the actuators are operational, but also when some of them experience failure.

To accomplish this goal, the method of multiple Lyapunov functions is used to analyze the IS stabilization. This approach results in solving a finite number of Riccati-like matrix equations to obtain the feedback control laws for each mode, which includes some tuning parameters to reduce the conservativeness of the control design. Simultaneously, to properly orchestrate the jump among the system modes, the switching moments are determined by the average dwell-time switching rule.

Finally, some numerical examples with simulations are presented to clarify the proposed theoretical results.

## Abstract

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In this study, a ratio dependent diffusive predator – prey model with Holling - Tanner type functional response with delay is investigated. The local stability of a positive equilibrium and the existence of Hopf bifurcations are established. By using the normal form theory and center manifold theorem, the explicit algorithm determining the stability and direction of the bifurcating periodic solutions are derived. The numerical simulations are also performed to justify the theoretical results.

# SS-OCDG Optimal Control and Differential Games

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# A Dynamic Model of the Limit Order Book

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A bidding game related to a continuum model of a one-sided Limit Order Book (LOB) was recently considered in [1, 2, 3, 4], proving the existence and uniqueness of a Nash equilibrium and determining the optimal strategies for the various agents. In the basic model, it is assumed that an external buyer asks for a random amount $X > 0$ of a given asset. This amount will be bought at the lowest available price, as long as this price does not exceed some (random) upper bound $\overline{P}$. Several sellers offer various quantities of this same asset at different prices, competing to fulfill the incoming order, whose size is not known a priori. It is shown as Figure 1.

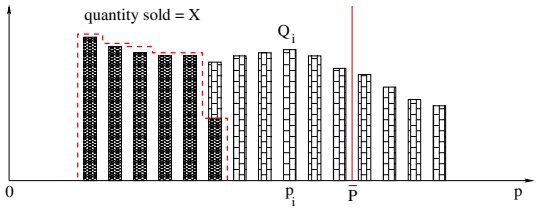


Figure 1: An external buyer will buy a random quantity $X$, at the lowest available price, as long as it does not exceed a3 upper bound $\overline{P}$

Having observed the prices asked by his competitors, each agent must determine an optimal strategy, maximizing his expected payoff. Because of the presence of the other sellers and of the upper bound $\overline{P}$ on the acceptable price, asking a higher price for an asset reduces the probability of selling it. As a consequence, a unique shape of the LOB is determined, which represents a Nash equilibrium between the various agents.

The models considered in [1, 2, 3, 4] all have the form of a “one shot game", with one side of the LOB. All players’ payoffs are completely determined as soon as one single incoming order is received.

This time, we consider an equilibrium model of the Limit Order Book in a stock market, where a large number of competing agents post “buy" or “sell" orders. For the “one-shot" game, it is shown that the two sides of the LOB are determined by the distribution of the random size of the incoming order, and by the maximum price accepted by external buyers (or the minimum price accepted by external sellers). We then consider an iterated game, where more agents come to the market, posting both market orders and limit orders. Equilibrium strategies are found by backward induction, in terms of a value function which depends on the current sizes of the two portions of the LOB. The existence of a unique Nash equilibrium is proved under a natural assumption, namely: the probability that the external order is so large that it wipes out the entire LOB should be sufficiently small.

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# An Optimal Control Approach to Structured Treatment Interruptions for HIV Patients

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Highly Active Antiretroviral Therapy (HAART) has changed the course of HIV treatments since its introduction. Under HAART, viral load decreases exponentially in the weeks after the start of treatment and is maintained at low levels so long as treatment is continued. Despite this exponential decline in viral load, these treatments do not completely clear the virus from the patient, and a life long therapy is necessary to maintain low viral load. Even with this kind of success, the best way to treat acutely infected HIV patients is still an open question with many approaches under investigation. For many patients, long term continuous HAART is expensive and can include problems with drug toxicity and side effects, as well as increased drug resistance. It has been shown that approximately 80% of patients who adhered to less than 70% of the prescribed treatment regimen experienced treatment failure, whereas patients of high adherence (>95%) experienced the best results. Long term use of protease inhibitors has been associated with insulin intolerance, cholesterol elevation, and the redistribution of body fat. Because of these reasons, some HIV infected patients will voluntarily terminate HAART. Some of these patients will also interrupt the continuous prescribed therapies for short or long periods. After discontinuing HAART, patients will usually experience a rapid increase in viral load coupled with a immediate decline in $CD4^+$ counts.

The canonical example of a patient undergoing unsupervised breaks in HAART is that of the “Berlin patient". In this case, the patient was able to control viral load in the absence of treatment by cycling HAART on and off due to non-related infections. When treatment was fully stopped after day 176, the patient’s viral load did not immediately rebound as is consistent with going off treatment. Due to this patient, interest in the use of structured treatment interruptions (STI) as a mechanism to regulate an HIV infection piqued.

One of the key variables in the design of any STI based protocol is the criteria in which patients are removed or placed back on treatment. In some studies the viral load was the primary indicator as to when treatment would resume, whereas in other studies off periods were of a fixed length, followed by a fixed length on period. The former approach is simpler, but harder to administer as it requires a higher level of patience scrutiny with more expensive and inconvenient blood tests. The latter strategy is easier to implement in larger patient groups, but the on/off periods are still up for debate and the subject of many clinical trials. Currently the period durations are determined either in an ad-hoc style, or by trying to adapt the methodologies of other trials.

In this talk, we use a mathematical model of HIV dynamics that has been validated using clinical data to determine optimal STI regimes. The optimal STI was implemented in the context of the receding horizon control (RHC). Since RHC is a feedback control, it allows for adjustment for unexpected perturbations to the treatment schedule, e.g. the patient decides to go off-treatment for a period of time not otherwise prescribed.

# APPLICATION OF EULER'S METHOD FOR THE SOLUTION OF OPTIMAL CONTROL PROBLEMS

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**Abstract**

*The fact remains that various authors has worked extensively on finding approximate solutions to continuous optimization problems (i.e. optimal control problems) which has a numerous applications in engineering, social sciences and even management sciences etc. many of this authors constructed control operators which was tested on their own built algorithms to be employed for the solution of this class of problems. But in this paper, we employed a method called Euler Equation which is aimed at taking care of this same class of problems. The authors of this paper desire that, with the derivation of the Euler Equation, one will circumvent the difficulties undergone in constructing any kind of control operators and its application will further improve the result of the existing methods in solving this class of problems.*

**Keywords:** *Control Operator, Euler's Method and Optimal Control Problems.*

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# Conservation laws and some applications to traffic flows

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In this talk, I will introduce a new class of models of traffic flow on a network of roads. In these models, the percentage of drivers who travel along an incoming road and wish to turn into an outgoing road is not a constant. Moreover, the drivers who enter a congested road are placed in a buffer of limited capacity, waiting their turn in line. The main goal is to describe traffic flow at intersections and study optimization problems on a network of roads.

I will present the well-posedness result for a new intersection model of traffic flows, and the existence of globally optimal solutions, Nash equilibrium solutions for a decision problem involving a continuum of drivers on the network.

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## GROWTH MODEL FOR TREE STEMS AND VINES

In this talk, we propose a model describing the growth of tree stems and vine, taking into account also the presence of external obstacles. The system evolution is described by an integral differential equation which becomes discontinuous when the stem hits the obstacle. The stem feels the obstacle reaction not just at the tip, but along the whole stem. This fact represents one of the main challenges to overcome, since it produces a cone of possible reactions which is not normal with respect to the obstacle. However, using the geometric structure of the problem and nonlinear analysis tools, we are able to prove existence and uniqueness of the solution under natural assumptions on the initial data.

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# Induced optimization for PDE constrained optimal control problems with linearly appearing control variable

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We consider optimal control problems subject to PDE constraints where the control variable appears only linearly. This type of problem occurs in many applications but provides several theoretical and numerical difficulties when regularization terms are neglected since the resulting controls can be bang–bang or singular.

In optimal control for ODEs, the so–called induced optimization approach provides an efficient method for the numerical solution as well as a convenient possibility for the verification of sufficient optimality conditions and the application of sensitivity analysis in the class of controls with the same control structure [3]. For bang-bang controls with certain regularity properties, even the optimality in the class of all possible controls is ensured [2].

In this talk, we extend the ODE approach to certain problems with PDE constraints. For a parabolic problem with boundary control [1], we discuss optimality conditions in the induced problem by regarding variational derivatives of the states as well as of the Lagrangian function with respect to switching times. Similarly to the ODE case, the state variations satisfy certain initial value problems which can be used to show that the Lagrangian variations depend only on state variations of one order lower.

The results will be illustrated by numerical examples where, by semi–discretization in space, the connection to ODE problems can be observed. Finally, a challenging application of a nonlinear battery model with a state constraint [4] will be treated numerically by our method.

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# New Approach for Modelling of Large Scale Engineering Systems

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Engineering systems are becoming increasingly difficult as the man organized systems are growing complex. All models are simplifications and abstractions of real world problems. If done correctly, then the idealization provides a useful approximation of real situation, or at least certain parts of real situations. The interconnection of artificial intelligence (AI) techniques and the multitarget tracking has applications in both military and civilian areas.

A great deal of interest in the field of (AI) has generated recently the success of widely published computer software systems. The high-quality performance of these systems in areas heretofore considered too complex for conventional programming techniques has given rise to Expert Systems(ES).

The development of an (ES) generally includes the following: analysis, design, implementation testing, user acceptance, and maintenance.

A new approach is given when creating the random input flow in the searching area of an intelligent aerospace system. The model is described by parameters as waiting time, time of stay inside the system, searching time, and service time. Targets flow are without consequences, i.e. probability of arrival of new targets are not depending on previous situation.

The designed model can be used or enlarged for solution of some aerospace and traffic control systems.

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# Optimal Control in Poro-Visco-Elastic Models

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Fluid flows through porous deformable media find many applications in biology, medicine and bioengineering, including tissue perfusion and fluid flow inside cartilages and bones. These fluid-solid mixtures are described mathematically by nonlinear poro-visco-elastic systems in bounded domains, characterized by (i) strong coupling through permeability described as a nonlinear function of volumetric solid strain, and (ii) non-homogeneous Dirichlet and Neumann boundary conditions on both elastic displacement and fluid pressure. The recent work in [2] provides a theoretical and numerical analysis for these coupled systems, and identifies the time regularity of the imposed boundary traction as a crucial factor that guarantees boundedness of the solutions. Moreover, the study in [2] shows that the system dynamics fundamentally change as visco-elastic effects vanish. This is very important, as it is known that visco-elastic properties of biological tissues often vary with age, health, and disease. Motivated by these new results, we performed numerical sensitivity analysis on these models with respect to boundary data and structural visco-elasticity in [1]. Our findings show that the solution is more sensitive to boundary traction in the elastic case than in the visco-elastic scenario and that the effects of the boundary source are most significant for the Darcy fluid velocity. Currently, we are investigating optimization and optimal control problems subject to poro-visco-elastic models, in connection with perfusion in the optic nerve head and its connections to the development of glaucoma.

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# Optimal control of breast cancer : Investigating estrogen as a risk factor

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Breast cancer is the most common cancer in women both in the developed and underdeveloped world. In this study, we present a system of four ordinary differential equations which consider population dynamics among normal cells, tumor cells and immune response. Additionally, we consider the effects of excess estrogen, immune booster on the above mentioned cell populations. However, optimal control theory is applied to investigate optimal strategies for controlling the spread of cancerous cells using treatment; anti-cancer and ketogenic diet as the system control variables. To also check the impact of using combinations of the two controls or one at a time on the tumor metastasis.

**Keywords:** Breast Cancer, Optimal control, Maximum principle, Ketogenic diet

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# Optimal control of systems with evolving dynamics

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This talk is dedicated to a new class of problems of optimal control of dynamical systems under uncertainty. We start with problems of optimal control of systems in which uncertainty is modelled in terms of some scenarios of evolution of system's dynamics. The main dificulty in study of such problems lies in the fact a that bifurcating structure of possible scenarios requires an application of non-anticipating (causal) control procedures.

We describe optimization theory of characterization of such optimal non-anticipationg strategies. Assuming that the set of possible evolution scenarios is finite and is known along with probabilities of realization of such scenarios, we derive necessary conditions for optimal non-anticipating strategies in terms of some non-standard maximum principle. The main feature of this maximum principle is new adjoint system which is significantly different from the one in classical Pontryagin maximum principle.

We demonstrate that these new optimality conditions can be used for a construction of optimal discontinuous feedback control. Robustness properties of this feedback with respect to small measurement errors of state vector and small perturbations of the dynamics are also studied.

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# Time-optimal Control Problems in the Space of Probability Measures and the Superposition Principle

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This talk aims to discuss generalizations of time-optimal control problems in the space of probability measures with finite $p$-moments endowed with the topology induced by the Wasserstein metric $W_p$, $(\mathscr{P}_p(\mathbf{R}^d), W_p)$, with $p \geq 1$, and to give an insight on the main tools used.

The main motivations to pass from the analysis of finite-dimensional control problems to their macroscopical counterparts in $\mathscr{P}_p(\mathbf{R}^d)$ are the following. On one hand we want to model realistic situations in which the occurence of noise only allows a probabilistic knowledge of the state of the system; on the other hand, the modeling of multi-agent systems demands a statistical description of the evolving mass of agents/particles.

In a mass-preserving context, the time-evolution of a given initial probability measure $\mu_0$ is given by a *controlled* continuity equation $\partial_t \mu_t + \mathrm{div}(v_t \mu_t) = 0$, where $v_t : \mathbf{R}^d \to \mathbf{R}^d$ has to be chosen among the $L^p_{\mu_t}$-selections of a given set-valued map $F$ governing the underlying dynamics of characteristics in the form of a differential inclusion. We assume the standard hypothesis on $F(\cdot)$, i.e. nonempty convex and compact values, continuity and linear growth. After providing a generalization of target set and the minimum time function, we briefly present some results as counterparts to the classical ones such as: Dynamic Programming Principle, existence of optimal trajectories, attainability and regularity results, and an HJB equation solved by our value function in some suitable viscosity sense.

Major attention will be given to the main tool used for these studies: the *Superposition Principle* by Ambrosio-Gigli-Savaré in [1] which gives a characterization of a (macroscopic) solution at time $t$ of the continuity equation, $\mu_t$, by using a (not-uniquely determined) probability measure $\eta$ concentrated on the integral solutions of the finite-dimensional underlying ODE.

We finally prove an extension of the Superposition Principle for differential inclusions. The idea is to build up a measure $\eta$ concentrated on Carathéodory solutions of the differential inclusion which can thus possibly cross each other. This measure $\eta$ results in a probabilisitic representation for a solution $\mu_t$ of a continuity equation. Its driving velocity field evaluated at a point $x \in \mathbf{R}^d$ turns out to be the integral average w.r.t. $\eta$ of the underlying admissible vector fields crossing position $x$ at time $t$. This tool can be applied to improve the previous study and in crowd dynamics models.

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# The Vanishing Viscosity Limit for a System of H-J Equations Related to a Debt Management Problem

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We study a system of Hamilton-Jacobi equations with discontinuous coefficients

$$(r+\rho(x))V \;=\; H(x,p(x),V'), \tag{1}$$

together with a family of smooth viscous approximations

$$r+\rho(x))V_n \;=\; H(x,p_n(x),V_n')+\frac{\sigma_n^2 x^2}{2}V_n''. \tag{2}$$

The main motivation comes from a problem of optimal debt management, in infinite time horizon, with exponential discount and a bankruptcy risk. As in Refs. [1, 2, 3, 4, 5], this is modeled as a noncooperative game between a borrower and a pool of risk-neutral lenders. The scalar equation Eq. (1) is supplemented by an additional ODE for the function $p$

$$\rho(x)\,(p-\theta(x)) = (r+\lambda)(1-p)+H_\xi(x,V',p)p', \tag{3}$$

and the Hamiltonian function in Eqs. (1,2,3) is defined as

$$H(x,p,\xi) \;\doteq\; \min_{\omega\in[0,1]}\left\{L(\omega)-\frac{\xi}{p}\omega\right\}+\xi\left(\frac{\lambda+r}{p}-\lambda\right)x+\rho(x)B. \tag{4}$$

In Ref. [2], we first construct a solution to the second order equation Eq. (2), which can be interpreted as a Nash equilibrium solution to a differential game with stochastic dynamics. Then we study the limits $V_n \to V$ and $p_n \to p$ as the diffusion coefficient $\sigma_n \to 0$. Due to the possible discontinuity of $p$, the Hamiltonian in Eq. (1) is discontinuous w.r.t x and thus the analysis becomes nonstandard. Furthermore, since we are modeling a game, the hamiltonian function for the borrower is not given a priori, but is determined by the optimal reply adopted by the lenders. In turn, this reply depends on the feedback control chosen by the borrower. Our main result shows that under suitable assumptions, this limit yields a solution to Eq. (1) and determines an equilibrium solution to a differential game with deterministic dynamics.

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# SS-RAWP Recent Advances in Mathematical and Computational Aspects of Wave Propagation

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# A compact alternative directional implicit method for solving two-dimensional fractional acoustic wave equation

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Seismic wave equations have been widely used in modelling wave propagation. Recently there has been increasing interest in using fractional acoustic wave equation to accurately characterize wave propagation in attenuation medium [6]. It is believed that inclusion of fractional time derivative in seismic wave equation will better model the attenuation and dispersion in complex media[1]. However numerical solution, especially highly accurate numerical solution of such acoustic wave equation is a fairly challenging computational task. So far very few work has been reported on the numerical solution of the fractional acoustic wave equation, in particular for 2D and 3D cases. In this work we consider the following two-dimensional acoustic wave equation with fractional time derivatives

$$ {}_0^C D_t^{1+\alpha} u = c^2 \Delta u + f(x,y,t), \qquad (x,y) \in \Omega, \;\; 0 < t \le T, \;\; 0 < \alpha < 1, \tag{1} $$

with the initial condition

$$ u(x,y,0) = u_0(x,y), \quad u_t(x,y,0) = v_0(x,y), \quad (x,y) \in \Omega $$

and boundary condition

$$ u(x,y,t) = \psi(x,y,t), \qquad (x,y) \in \partial\Omega, \;\; 0 < t \le T, $$

where the fractional derivative ${}_0^C D_t^{1+\alpha} u$ is defined by

$$ {}_0^C D_t^{1+\alpha} u = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial^2 u(x,y,s)}{\partial s^2} \, ds. $$

On the other hand, several efficient and accurate compact finite difference methods have been developed to solve fractional diffusion equations, in one-dimensional and multi-dimensional spaces[2, 3, 4, 5]. Based on these methods, we developed a compact higher-order alternative directional implicit method to solve the fractional acoustic wave equations given in Eq. (1). Several numerical examples were solved to demonstrate the efficiency and accuracy of the new methods.

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**Abstract**

Hyperbolic conservation laws are a class of partial differential equations that model wave propagation. Nonlinear problems can exhibit wave steepening and shock formation. The latter phenomenon can lead to instabilities and oscillations in high-order numerical methods due to Gibbs' phenomenon. Stabilization of these numerical oscillations can be achieved through slope limiting. For one dimensional problems, slope limiters that ensure a total variation diminishing property have been popular. In two dimensions, methods that enforce this property are at most first order. In this talk we propose a two-dimensional slope limiting procedure on unstructured triangular meshes for the modal discontinuous Galerkin finite element method. This limiter enforces a local maximum principle, which guarantees L-infinity stability in the means, and is still second order accurate.

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# Asymptotic stability in the variable-speed $\phi^4$ model: odd perturbations

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The $\phi^4$ model is a classical nonlinear equation that arises in quantum field theory, statistical mechanics, and other areas of physics. (See e.g. [5].) We are interested in the case where the propagation speed $c$ is allowed to vary with position. The equation is given in one space dimension by

$$\partial_t^2\phi - c^2(x)\partial_x^2\phi = \phi - \phi^3, \quad (t,x) \in \mathbb{R}\times\mathbb{R}, \tag{1}$$

where $c(x)$ is a uniformly positive function. We restrict our attention to even functions $c$ that are small deviations from the constant unit speed $c \equiv 1$. The focus of this study is the long-time behavior of (1), in particular the stability of the stationary solution connecting the two minima of the potential $\frac{1}{4}(1-\phi^2)^2$. In the case $c(x) \equiv 1$, this stationary solution, called the *kink* is known explicitly: $H(x) := \tanh\left(x/\sqrt{2}\right)$. The kink in the $\phi^4$ model is seen as a prototype for solitons that occur in more complicated field theories (see [5]). Using fixed-point methods, we can show the existence of a kink-type solution $K(x)$ for suitable non-constant $c(x)$. The existence proof also yields important information (odd parity and an explicit decay rate) about $K$.

Our main result [6] is the asymptotic stability of $K(x)$ with respect to odd perturbations in the natural energy space. This extends the recent work of Kowalczyk, Martel, and Muñoz [1], who proved asymptotic stability in the case $c \equiv 1$, again in the case of odd perturbations. Their approach is partially based on the work of Martel and Merle on generalized KdV equations [2, 3] and Merle and Raphael [4] on the mass-critical nonlinear Schrödinger equation, but was adapted to additional difficulties resulting from the exchange of energy between internal oscillations and radiation, and the different decay rates of the corresponding components of the solution. (See also the work of Soffer and Weinstein [7] on general Klein-Gordon equations with potential.) To extend this approach to the variable-speed case, it is necessary to understand the spectrum of the linearization around the variable-speed kink $K(x)$. In the constant-speed case, the linear operator and its spectrum are known explicitly, but in our case a detailed perturbative analysis is required.

Time permitting, we will discuss ongoing work on the extension of this study to non-perturbative speeds $c(x)$.

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# Bifurcations of relative periodic orbits in NLS/GP with a three-well potential

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We consider the nonlinear propagation of solutions to the nonlinear Schrödinger/Gross-Pitaevskii equation

$$i\partial_t u = -\partial_x^2 u + V(x)u - |u|^2 u$$

in which the potential is given as the sum of three equally-spaced exponentially-localized wells $V(x) = V_0(x-L) + V_0(x) + V_0(x+L)$ with $L \gg 0$. This system is known to support nine different stationary time-harmonic solutions which arise in various bifurcations as a parameter $N$, the squared $L^2$ norm is raised. We consider the relative periodic orbits that occur due to some bifurcations in this system, including Hamiltonian Hopf bifurcations and saddle-node ($0^2 i\omega$) bifurcations; see figure 1. We derive a finite-dimensional reduction of the equations to a small Hamiltonian system of ODE, to which we apply Hamiltonian normal form methods. These allow us to uncover and explain the existence and bifurcations of families of relative periodic periodic orbits. Careful numerical experiments confirm this for the ODE system and shows that such structures are mimicked by solutions to the underlying NLS/GP system.

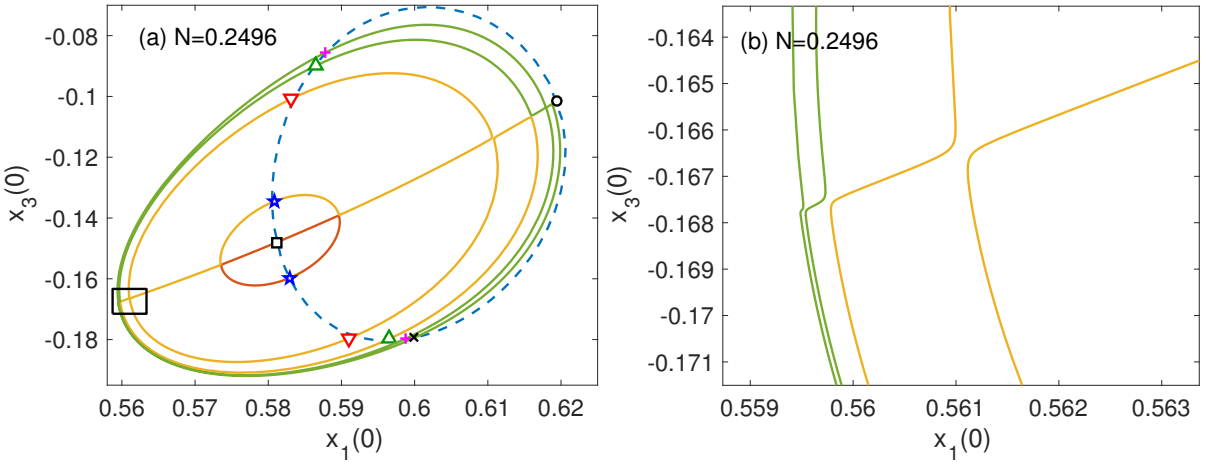


Figure 1: (a) Branches of relative periodic orbits arising due to a $0^2 i\omega$ bifurcation in a finite-dimensional model of NLS-GP orbits. (b) A close-up showing complex pseudo-intersection structure of these branches.

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**Birkhoff normal form for nonlinear wave equations**

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Abstract: Many theorems on global existence of small amplitude solutions of nonlinear wave equations in $\mathbb{R}^n$ depend upon a competition between the time decay of solutions and the degree of the nonlinearity. Decay estimates are more effective when inessential nonlinear terms are able to be removed through a well-chosen transformation. Additionally, most physically relevant wave equations can be formulated as Hamiltonian PDEs, and the analysis of their solutions can be considered in this context. In this talk, we construct Birkhoff normal forms transformations for the class of wave equations which are Hamiltonian PDEs and null forms, using the flow of an auxiliary Hamiltonian system . This gives a new proof via canonical transformations of the global existence theorems for null form wave equations of S. Klainerman and J. Shatah in space dimensions $n \geq 3$. The case $n = 2$ is also under consideration, which involves a normal forms interpretation of modified scattering. These results are work-in-progress with A. French and C.-R. Yang.

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# Estimates for spectral multipliers

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This talk will be about several estimates we have recently obtained for equations with Hamiltonian

$$H = -\Delta + V$$

in dimension three and for potentials $V$ of approximately critical (inverse square) decay. These include resolvent kernel bounds, Mihlin multiplier bounds, Strichartz estimates, Gaussian and Poisson kernel bounds, and others.

Unlike in many such results, we are not assuming the absence of negative energy bound states.

Note for the organizers: This is just one possibility; the topic of my talk may change by then.

**Title**: Fermi's Golden Rule and $H^1$ Scattering for Nonlinear Klein-Gordon Equations with Metastable States

**Abstract**: Due to a nonlinear Fermi golden rule, the excited states for Klein-Gordon equations are unstable under a nonlinear perturbation. The outcomes of this instability are the metastable states. We will derive an anomalously slow-decaying rate (with both upper and lower bounds $1/(1+t)^{1/4}$) for these metastable states. Even though a sharp lower bound is obtained, we further show that $H^1$ scattering still holds.

In this talk we will discuss our past and recent results regarding the problem of acoustic and electromagnetic field manipulation with the help of exterior surface active sources. We will first present a series of smooth scalar control results for the Helmholtz equation and based on these results we will describe our strategy for electromagnetic field control. Applications to scattering cancellation, near-field field synthesis ( in free space and waveguides) and inverse source problems will be discussed as well.

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# Field patterns in space-time microstructures

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Field patterns [1] are a new sort of wave that occur in space-time microstructures with a geometry chosen such that a disturbance does not generate a complicate cascade of subsequent disturbances, but rather concentrates on a pattern of characteristic lines. This pattern is the field pattern. In one spatial direction plus time, the field patterns occur when the slope of the characteristics is, in a sense, commensurate with the space-time microstructure. For instance, in [2] we propose two examples of space-time geometries in which field patterns occur: they are two-phase microstructures in which rectangular space-time inclusions of one material are embedded in another material. After a sufficient large period of time, the field patterns in both microstructures have local periodicity both in time and space, due to the PT–symmetry of the chosen space-time geometries. This allows one to focus only on solving the problem on a discrete network and to define a suitable transfer matrix that, given the solution at a certain time, provides the solution after one time period. Many of the eigenvalues of this transfer matrix have unit norm and hence the corresponding eigenvectors correspond to propagating modes. However, there are also modes that blow up exponentially with time coupled with modes that decrease exponentially with time. Examples of space-time microstructures such that the transfer matrix only has eigenvalues on the unit circle, so that there are no growing modes (modes that blow-up) are presented in [2]: they are space-time checkerboards in which the wave speeds of the components satisfy special relations. Interestingly, when there is no blow-up, the waves generated by an instantaneous disturbance at a point look like shocks with a wake of oscillatory waves. This sets an arrow of time in the sense that it would be extremely difficult to produce the initial conditions necessary to create the corresponding time-reversed waves.

Besides opening new avenues of research regarding wave propagation in space-time microstructures, the theory of field patterns is particularly interesting also for some of its features which hint at a possible connection with quantum mechanics: field patterns exhibit both a particle-like aspect and a wave-like aspect, as they are propagating waves concentrated on lines in a space-time diagram. Furthermore, even though they appear in scalar wave equations, they have a multidimensional or multicomponent nature. In fact, in the linear model we developed in [1], field patterns with different spatial shifts do not interact, but rather evolve as if they lived in separate dimensions (as many dimensions as the number of field patterns), with each dimension playing the same role of the others, as do the different dimensions associated with say the multielectron Schrödinger equation with noninteracting electrons.

Moreover, the theory of field patterns could be very useful in the study of spatially periodic composites of hyperbolic materials. In fact, in the limit where the loss goes to zero, a two-dimensional spatially periodic hyperbolic material can be viewed as a space-time microstructure in one spatial dimension plus time, if one reinterprets one of the two spatial coordinates as time. Therefore, the results obtained within the theory of field patterns may be applicable to hyperbolic materials in the limit where the imaginary part of the dielectric tensor goes to zero.

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# Global Existence of Weak Solutions for the Burgers-Hilbert Equation

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Consider the Burgers-Hilbert equation

$$u_t + \left(\frac{u^2}{2}\right)_x = \mathbf{H}[u], \tag{1}$$

where $\mathbf{H}[f](x) \doteq \lim_{\varepsilon\to 0+} \frac{1}{\pi}\int_{|y|>\varepsilon} \frac{f(x-y)}{y}\,dy$ denotes the Hilbert transform of a function $f \in \mathbf{L}^2$. This equation was derived by J. Biello and J. Hunter from a model for nonlinear waves with constant frequency ([1]). For sufficiently smooth initial data the local existence and uniqueness of solutions of (1) was proved in [2], together with an estimate on the time interval where the solution remains smooth. Here we are mainly concerned with existence and uniqueness of entropy weak solutions globally in time.

This talk will present some recent results. Namely: the global existence of entropy weak solutions, a priori estimates in $\mathbf{L}^2$ and in $\mathbf{L}^\infty$, and a uniqueness result in the spatially periodic case.

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# Linear stability of the catenoid under the VMC flow outside of symmetry

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In a previous paper [2] we examined the stability of the catenoid under the vanishing mean curvature (VMC) flow in Minkowski space, under the assumption that the perturbations exhibit both axial symmetry and reflection symmetry. The main difficulty there is the presence of a negative potential in the linearized dynamics which drives a one-dimensional exponential instability. Our result showed that the negative potential is the only source of instability under our symmetry assumptions.

In this talk we analyze the situation for the linearized dynamics outside of the symmetry class. We show that the higher angular momentum perturbations exhibit (uniform) dispersive decay. The method used is a modification of the methods used in [1], and can be applied to large classes of linear wave equations with potentials on warped product space-times.

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# New Source Models for Radiation from Thin Wire Antennas

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The problem of evaluating the current distribution that is induced on a thin straight wire antenna by a given axial electric field was first described by Pocklington [1] more than a century ago. Indeed, if the centerline of a wire of radius $a$ lies on the interval $z \in [-1,1]$, then the current $J(z)$ induced by an incident electromagnetic field with wave-number $k$ and axial component $e(z)$ can be obtained as a solution of the Pocklington equation

$$\left(\frac{\partial^2}{\partial z^2} + k^2\right) \int_{-1}^{1} G(z-t)\, J(t)\, dt = -4\pi i k e(z) \tag{1}$$

subject to the end-point conditions $J(-1) = J(1) = 0$. The differential operator in (1) can inverted to obtain the well-known Hallén formulation

$$\int_{-1}^{1} G(z-t)\, J(t)\, dt = \alpha_1 \cos kz + \alpha_2 \sin kz - 4\pi i \int_{-1}^{z} e(t) \sin[k(z-t)] dt. \tag{2}$$

We denote $G(z)$ as the well-known thin wire kernel (see e.g. [3]) and constants $\alpha_1$ and $\alpha_2$ are chosen so as to ensure the end-point conditions are satisfied. Interestingly, equation (2) was derived by Erik Hallén [2] to specifically treat the case when a delta source lies on the wire; i.e., $e(z) = V\delta(z)/(2\zeta_0)$, where $\zeta_0$ the impedance of free space. The Dirac delta function arises as a finite potential difference $V$ is imposed over an infinitesimal distance (or gap) at the origin $z = 0$. The appearance of the delta function poses significant difficulties in producing accurate algorithms to treat this important problem, and yet the delta-gap is likely the most common source model in the literature.

We have recently developed a method to treat the singular terms associated with the delta function appearing in equation (2) to arbitrarily high order. The resulting numerical scheme to compute the current $J(z)$ is quickly convergent, and radiated fields are easily evaluated as part of the post-processing of the solution. We give several numerical examples illustrating the convergence rates achieved by our code and the improvements it offers over classical approaches. Our solvers are easily extended to treat another source models, e.g. the magnetic frill generator [4], and several new source models which we propose as a part of this work. We present the sketch of a rigorous mathematical proof that all of the source models we examine are essentially equivalent.

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# Nonlinear waves in nonlinear Schrödinger (NLS) systems

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**Abstract**

In this talk, we will present a two-component NLS system in one and two spatial dimensions. The formation of bright solitonic bound states in the second component will be discussed and their bifurcation points will be identified by the underlying linear limit. This way, nonlinear states can be identified and their stability will be studied. Finally, a novel continuation method, the so-called, deflated continuation will be discussed together with its applicability towards identifying states in NLS systems.

**Title**: On Gravitational Collapse in General Relativity

**Abstract**: In the process of gravitational collapse, singularities may form, which are either covered by trapped surfaces (black holes) or visible to far-away observers (naked singularities). In this talk, I will present results on both scenarios. For Einstein vacuum equations in $R^{3+1}$, with no symmetry assumptions, I construct spacetimes, showing that a black hole is emerging from a point. For Einstein vacuum equations in higher dimensions, together with Xuefeng Zhang, we construct singularities, which are not covered by a black hole region.

# Periodic traveling waves of the short pulse and Ostrovsky equations: existence and stability

Milena Stanislavova

**Abstract**

We consider the Ostrovsky and short pulse models in a symmetric spatial interval, subject to periodic boundary conditions. We construct various periodic traveling wave solutions of the short pulse equation - a family of traveling peakons with corner crests, as well as classical traveling waves in terms of Jacobi elliptic functions. In both cases, we show spectral stability, for all values of the parameters. This is achieved by studying the non-standard eigenvalue problems in the form $\mathcal{L}[u] = \lambda u'$, where $\mathcal{L}$ is a Hill operator. This is a joint work with S. Hakkaev and A. Stefanov.

Although many studies have been carried on to understand the Zakharov weak turbulence equation for capillary waves since its derivation in the 60s, the question about the existence and uniqueness of solutions to the equation remains unanswered, due to the complexity of the equation. After the production of the first Bose-Einstein Condensates (BECs), there has been an explosion of physics research on the quantum kinetic theory associated to BECs and their thermal clouds. In our talk, we will briefly describe the connection between quantum kinetic and weak turbulence theories. We will also discuss our result trying to answer the existence and uniqueness questions of the Zakharov equation, based on our recent tools developed for quantum kinetic equations.

The talk will be based on the results described on the blog: On the Mathematics of Dispersive Waves and Quantum Gases.

Radiative transfer theory for luminescent solar concentrators and solar cells

There have been recent advances in making highly-efficient photovoltaic solar cells and designing luminescent solar concentrators (LSCs). I will review these applications and some of the mathematical challenges that arise in these fields. In particular, I will describe a radiative transport theory for LSCs, efficient computational methods to solve it, and its extension to photovoltaic solar cells.

# Random data Cauchy theory for power type nonlinear wave equations on $\mathbb{R}^d$

**Dana Mendelson**

**Abstract.** In this talk, I will discuss the random data Cauchy theory for some power type nonlinear wave equations on Euclidean space. Local well-posedness for these equations is by now well understood for initial data of subcritical or critical regularities, but techniques break down for initial data in the supercritical regime. In recent years, probabilistic methods have been used to investigate the behavior of solutions in regimes where deterministic techniques fail. I will present an almost sure global existence result in the supercritical regime for these equations, and a recent result on scattering for the energy critical equation in 4D with randomized radial data. I will discuss the main aspects of the proof, in particular, the randomization procedure for initial data in Sobolev spaces of low regularity, some new large deviation estimates, and energy estimates for a forced wave equation.

This talk is based on several joint works with Jonas Luhrmann, and work with Ben Dodson and Jonas Luhrmann.

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# Secondary Bifurcations along the Ground State and First Excited State Branches in Nonlinear Schrödinger Equations with External Potential

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I will discuss very recent results regarding the emergence of new bound state branches from ground states and excited states in nonlinear Schrödinger equations (NLS). Ground states and excited states have been known to bifurcate from the trivial (zero) solution under certain spectral assumptions on the external potential. The secondary bifurcations occur away from zero on these branches. First, I will present methods to investigate both the existence of these bifurcations at small amplitudes and the stability of the emerging branches. This is joint work with Hee Yeon Kim at University of Illinois. Then, I will discuss extensions of these results to large amplitudes. This is work in progress involving many collaborators that will be mentioned in the presentation.

We consider the Whitham equation on the whole line. Due to the smoothing nature of the linear operator, the question for existence of traveling wave solutions has been open till recently. In 2012, Ehrnstroem-Groves-Wahlen (EGW) have constructed such waves, but only for values of $c$ slightly bigger than one, even though the admissible range of wave speeds is $c \in (1, 2)$. The approach in EGW consists of a tour de force calculus of variations, supplemented by a bifurcation argument from the small KdV waves. Note that the EGW waves are of small amplitude.

In this work (joint with M. Ehrnstroem), we construct a one parameter family of such waves, with wave speeds $c \in (1, c_0)$ for some limiting value $c_0$, not necessarily close to 1. We conjecture that the wave with speed $c_0$ is the maximal amplitude wave (i.e. the highest wave, with amplitude $c/2$) and there are no waves with wave speeds $c \in (c_0, 2)$. However, we still find some interesting objects in the interval $(c_0, 2)$.

The argument uses calculus of variation construction, very different than the one employed by EGW. It is based on constraints on appropriately selected Orlicz spaces. Finally, all our traveling waves are shown to be bell-shaped, confirming the available numerical evidence. I will also speculate a bit about their stability as they are constructed as ground states of the appropriate constrained maximization problems.

# Spectral Stability of Solitary Traveling Waves in Hamiltonian Lattices and an Energy Criterion

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In this work, we provide different perspectives for studying the spectral stability of solitary traveling waves in Hamiltonian nonlinear dynamical lattices, which include examples such as granular crystals, the Fermi-Pasta-Ulam and the Toda lattice. First we consider an eigenvalue problem for a stationary solution in a co-traveling frame, while a traveling wave can also be viewed as a periodic orbit modulo shifts. We connect the eigenvalues of the former with the Floquet multipliers of the latter and introduce two equivalent approaches for studying the spectral stability.

We derive an energy-based spectral stability criterion which states a sufficient (but not necessary) condition for a change in the wave stability occurs when the functional dependence of the energy (Hamiltonian) $H$ of the model on the wave velocity $c$ changes its monotonicity. Moreover, near the critical velocity where the change of stability occurs, we provide explicit leading-order computation of the unstable eigenvalues, based on the second derivative of the Hamiltonian at the critical velocity $H''(c)$. We corroborate this conclusion with a series of analytically and numerically tractable examples and discuss its parallels with a recent energy-based criterion for the stability of discrete breathers. We also mention the close connection between this criterion and those exist for discrete breathers and solitary waves in continuum systems.

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# A numerical study on the importance of the trumpet's initial bore geometry

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Previously in [1], we examined the consequences of neglecting spatial dimensions in musical instrument simulations. We did this by numerically solving the equations of motion found in gasdynamics via the discontinuous Galerkin method (DGM) to simulate nonlinear sound wave propagation in a trumpet. Our results demonstrated that reducing the dimensionality of the problem was inadequate to model the spreading of the waves in all directions.

Since completing this work, we have studied the importance of properly modelling the bore geometry in-between the mouthpiece shank and first bend. We did this because less research has been done on this topic and it is often assumed that the bore prior to the bell is uniform in diameter (e.g., [2, 3]). However, close inspection near the mouthpiece revealed that the inner tubing before the first bend is more complex than alluded to by the outer geometry. We found that the radius of the trumpet bore 24 cm from the mouthpiece shank position is $2.12\times$ larger. Since volume increases by a factor of the radius squared, neglecting this variation could greatly influence the slope of the pressure entering the main body of the instrument and thus, how much the nonlinear waves distort inside the trumpet [4]. As part of our study, we again simulated nonlinear sound propagation in a trumpet using the DGM to numerically solve the three-dimensional compressible Euler equations. To validate our approach, we simulated the time-pressure waveforms of the previously recorded $B_3^b$ and $B_4^b$ musical notes played at *forte*. In particular, these pressure measurements obtained at the mouthpiece shank were prescribed as the boundary conditions on pressure (at the mouthpiece boundary of the computational trumpet) for the presented numerical simulations.

In our model, as done in [5], we assumed that losses due to visco-thermal effects were negligible. However, according to [6], for brass instruments, dampening can decrease the frequency (i.e., the pitch) of the lowest impedance peaks by approximately 5%. Furthermore, the amplitude of the frequency peaks (i.e., the volume) can be lowered by several orders of magnitude. To determine if our assumption was reasonable, we examined the difference between our simulations and experiment to see if the resulting spectral components of the simulated notes deviated from our experiment by the amounts suggested in [6]. Our analysis revealed however that for a realistic trumpet geometry, discrepancies were much smaller. Therefore, our results seem to indicate that the shape of the tube prior to the first bend must be modelled to obtain accurate results while neglecting losses; but, neglecting such losses is inadequate if one wants to model the trumpet with a simplified geometry.

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**The nonlinear Schrodinger equation on large domains (Zaher Hani)**

We will consider the nonlinear Schrodinger equation on a box of size L. We will be interested in the question of finding the effective dynamics in the limit of large L. The answer depends on the time scale over which we would like to describe the effective behavior. We shall discuss some of those time scales and the effective equations that describe the dynamics in each case. This is joint work with T. Buckmaster, P. Germain, and J. Shatah.

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# Travelling waves of a highly nonlinear fourth-order wave equation

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A highly nonlinear, fourth-order wave equation that models [1, 2, 3, 4] the continuum theory of long wavelength pulses in weakly compressed, discrete, homogeneous chains with a general power-law contact interaction is studied:

$$c^{-2}u_{tt} = u_x^{k-1}u_{xx} + \alpha u_x^{k-3}u_{xx}^3 + \beta u_x^{k-2}u_{xx}u_{xxx} + \gamma u_x^{k-1}u_{xxxx}, \quad k > 1. \tag{1}$$

For this wave equation, all solitary wave solutions and all nonlinear periodic wave solutions, along with all conservation laws, are derived [5]. The solutions are explicitly parameterized in terms of the asymptotic value of the wave amplitude in the case of solitary waves and the peak of the wave amplitude in the case of nonlinear periodic waves. All cases in which the solution expressions can be stated in an explicit analytic for m using elementary functions are worked out. In these cases, explicit expressions for the total energy and total momentum for all solutions are obtained as well. The derivation of the solutions uses the conservation laws combined with an energy analysis argument to reduce the wave equation directly to a separable first-order differential equation which determines the wave amplitude in terms of the travelling wave variable. This method can be applied more generally to other highly nonlinear wave equations.

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# SS-RPNMSC Recent Progress in Numerical Methods and Scientific Computing

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# A fourth-order compact numerical scheme for three-dimensional acoustic wave equation with variable velocity

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In this work we consider numerical solution to the following three-dimensional acoustic wave equation with variable wave velocity

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \Delta u + f(x,y,z,t), \qquad (x,y,z) \in \Omega, \;\; 0 < t \leq T, \tag{1}$$

with the initial conditions

$$u(x,y,z,0) = u_0(x,y,z), \qquad u_t(x,y,z,0) = v_0(x,y,z), \qquad (x,y,z) \in \Omega$$

and boundary condition

$$u(x,y,z,t) = \phi(x,y,z,t), \qquad (x,y,z) \in \partial\Omega, \;\; 0 < t \leq T,$$

where $c = c(x,y,z)$ is the spatially varying wave velocity.

Higher-order numerical solution of the above wave equation has been extensively used in various science and engineering applications, in particular in Geophysics for the purpose of prospecting exploration. One specific example is the seismic full waveform inversion problem, in which the acoustic wave equation is numerically solved ( forward modelling) for a large number of times during the iteration process.

Therefore, efficiency and accuracy of the numerical methods for solving the acoustic wave equation is critical in the success of seismic full waveform inversion. Despite the tremendous efforts that has been devoted during the past decades, it still remains a challenging task in the development of efficient and accurate finite difference method for multi-dimensional acoustic wave equation, especially for variable velocity case.

In this work, we extended the method [1] which combines the Padé approximation with Alternative Directional Implicit (ADI) method, to develop a fourth-order compact finite difference scheme to solve three-dimensional acoustic wave equation with variable velocity. To our best knowledge, this is the first attempt to develop fourth-order compact Padé scheme for acoustic wave equation in heterogeneous media. Numerical results show that the numerical method is accurate, efficient and stable.

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# A New Kind of Companion Matrix

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Investigating of a special companion matrix for the Mandelbrot polynomials that was invented by Piers W. Lawrence, we found that we could easily extend the construction to similar recursively-constructed polynomial families. After Donald Knuth asked us if we could do this for polynomials related to what he called "Euclid Numbers", i.e. $E_{n+1} = E_1, E_2 \ldots E_n + 1$, we discovered that we could. This led us to a general construction which gives a genuinely new kind of companion matrix. Apparently, that gives a new linearization for matrix polynomials, as well.

# A robust numerical method for the Maxwell equations with random interfaces

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A robust numerical method via the shape derivatives and low-rank approximation is developed for computations of three-dimensional Maxwell's equations with random interfaces. Based on a shape calculus, we estimate the statistical moments of the stochastic Maxwell equations in terms of perturbation magnitude. In order to capture the oscillations with high resolution near the interface, we adopt the adaptive edge element with third order polynomials to solve the deterministic equations approximating the expectation. For the second moment, an efficient low-rank approximation based on pivoted Cholesky decomposition is proposed to compute the two-point correlation function to approximate the variance of stochastic Maxwell's equations. Numerical experiments are presented to illustrate our theoretical results.

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# A wavelet based phase-field simulation of a two-phase flow in porous media

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In petroleum engineering, the displacement of oil by water is an improved oil recovery technique that is employed when primary oil production rates deteriorate. It is of great challenge to seek accurate, efficient, and robust numerical methods to simulate such a multiphase flow. In particular, numerical modelling of the capillary stress due to the steep variations of physical properties across a fluid-fluid interface remains elusive [1]. In this work, the Allen-Cahn phase-field method based on the van der Waals theory of free-energy has been considered to model the capillary stress [2], where the phase-field equation has been coupled with the volume averaged Navier-Stokes equation (see [3]). A goal of the present research is to develop a wavelet based methodology to characterize the immiscible displacement of two fluids in porous media.

Fig 1 demonstrates the accuracy of the phase-field simulation with respect to the small but finite values of the phase-field parameter, $0 < \varepsilon \ll 1$, when co-current to counter-current flow reversal occurs during the migration of the non-wetting phase in a porous medium. In addition to capturing the fluid-fluid interface accurately, the present phase-field simulation also demonstrates a good agreement with the experimental prediction of relative permeabilities in a porous medium. This talk aims to detail this novel numerical approach for simulating multiphase flow in porous media, and will discuss the potential of the phase-field method for the numerical simulation of oil reservoirs.

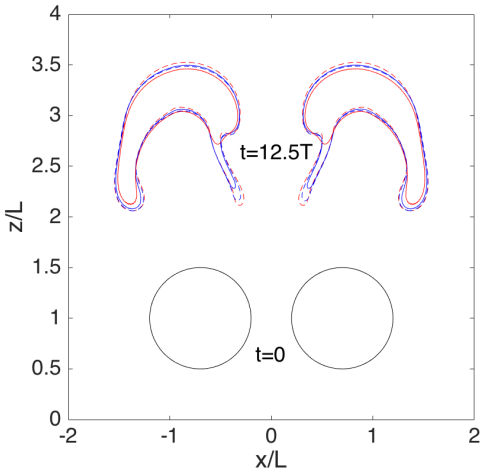


Figure 1: Phase-field simulation of two isolated bubbles of the non-wetting phase in a porous medium at $\varepsilon = 11.0 \times 10^{-3}$ (red –), $7.9 \times 10^{-3}$ (blue –), $5.6 \times 10^{-3}$ (blue – –), $2.5 \times 10^{-3}$ (red – –). The porous medium was saturated initially with the wetting phase. When co-current to counter-current flow reversal occurs, a finite value of $\varepsilon \in [2.5 \times 10^{-3}, 5.6 \times 10^{-3}]$ seems sufficient.

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# Comparative Study on Numerical Solutions of Partial Differential Equations

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***Abstract*—** There are many boundary value problems which involve partial differential equations. Only few of these can be solved can be analytical methods. In the most cases we depends on the numerical solution of such partial differential equations. The general linear partial differential equation of second order in two independent variables is of the form:

$$A(x,y)\frac{\partial^2 u}{\partial x^2}+B(x,y)\frac{\partial^2 u}{\partial x\partial y}+C(x,y)\frac{\partial^2 u}{\partial y^2}+F\left(x,y,u,\frac{\partial u}{\partial y},\frac{\partial u}{\partial y}\right)=0 \qquad ...(1)$$

Such a partial differential equation (1) may be elliptic $\left(if\ B^2-4AC<0\right)$, parabolic $\left(if\ B^2-4AC=0\right)$ or hyperbolic $\left(if\ B^2-4AC>0\right)$ according to its nature. In this paper, we compare the numerical accuracy of the solutions of elliptic type partial differential equations. Two Iterative numerical methods are compared, namely, Jacobi's Method and Gauss-Seidel Method. The comparison of accuracy is obtained through comparing the solutions of partial differential equations given by these two methods.

***Keywords*—** Partial Differential Equation, Jacobi's Method, Gauss-Seidel Method.

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# Convergence of approximation schemes for weakly nonlocal second order equations

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**Abstract**

A large number of interesting financial phenomena, continuous time games, motion by mean curvature, front propagation of surfaces, etc. are captured by nonlinear second order elliptic partial differential equations (PDEs). Such PDEs do not generally admit smooth solutions. As such, we look for other meaningful solutions, such as (nonsmooth) viscosity solutions. In order to compute viscosity solutions (e.g., via finite difference, volume, or element methods) one can invoke the seminal result that a monotone, stable, and consistent numerical scheme converges to the viscosity solution if the limiting PDE satisfies a maximum (a.k.a. comparison) principle. However, this result is established only for local PDEs and can be applied only to certain special nonlocal PDEs. In this talk, we extend this result to weakly nonlocal PDEs in a very general manner and give a financially motivated example from optimal stochastic impulse control.

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# Energy Law and Metamaterial Electromagnetic Computation

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The metamaterial with negative refraction index was first proposed in 1968 and constructed in 2000, which has brought a new revolution in electromagnetic and material science. Due to unusual physical properties that can not be found in natural materials, metamaterials have many important applications such as in aerospace application, aircraft radar and radio-frequency, microwave and wireless interconnect, nanolithography and medical imaging, cloaking device, and so on. In this talk, we will present our results on energy law of conservation of electromagnetic waves in metamaterials and the energy-preserving splitting FDTD methods for metamaterial electromagnetic computations. We will talk theoretical analysis results on energy conservation, stability and convergence of high-order accuracy of the developed schemes and will also simulate numerically the electromagnetic wave propagation in the DNG metamaterials whose results show the specific features of electromagnetic waves in metamaterials.

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# Error expansion for a symplectic scheme for stochastic Hamiltonian systems

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We consider the stochastic autonomous Hamiltonian system (SHS) in the sense of Stratonovich:

$$dP^i = -\frac{\partial H_0}{\partial Q^i}dt - \sum_{r=1}^{d}\frac{\partial H_r}{\partial Q^i}\circ dw_t^r, \quad dQ^i = \frac{\partial H_0}{\partial P^i}dt + \sum_{r=1}^{d}\frac{\partial H_r}{\partial P^i}\circ dw_t^r, \quad \mathbf{P}_0 = \mathbf{p}, \mathbf{Q}_0 = \mathbf{q}, \tag{1}$$

where $\mathbf{P}$, $\mathbf{Q}$, $\mathbf{p}$, $\mathbf{q}$ are $n$-dimensional column vectors, and $w_t^r$, $r = 1,\ldots,d$ are independent standard Wiener processes, for $t \in [0,T]$. The flow of (1) preserves the symplectic structure [1]. Moreover, the implicit scheme given by the following one step approximation preserves the symplectic structure and is of first weak order [1]

$$\bar{P}^i_{k+1} = \bar{P}^i_k - h\frac{\partial H_0}{\partial \bar{Q}^i} - \frac{h}{2}\sum_{r=1}^{d}\sum_{j=1}^{n}\frac{\partial}{\partial \bar{Q}_i}\left(\frac{\partial H_r}{\partial \bar{Q}_j}\frac{\partial H_r}{\partial \bar{P}_j}\right) - h^{1/2}\sum_{r=1}^{d}\frac{\partial H_r}{\partial \bar{Q}^i}\xi_{kr}, \quad \bar{\mathbf{P}}_0 = \mathbf{p} \tag{2}$$

$$\bar{Q}^i_{k+1} = \bar{Q}^i_k + h\frac{\partial H_0}{\partial \bar{P}^i} + \frac{h}{2}\sum_{r=1}^{d}\sum_{j=1}^{n}\frac{\partial}{\partial \bar{P}_i}\left(\frac{\partial H_r}{\partial \bar{Q}_j}\frac{\partial H_r}{\partial \bar{P}_j}\right) + h^{1/2}\sum_{r=1}^{d}\frac{\partial H_r}{\partial \bar{P}^i}\xi_{kr}, \quad \bar{\mathbf{Q}}_0 = \mathbf{q}. \tag{3}$$

Here $h = T/N$, everywhere the arguments are $(\bar{\mathbf{P}}_{k+1}, \bar{\mathbf{Q}}_k)$ and $(\xi_{kr})$ are i.i.d. random variables with the law $P(\xi = \pm 1) = 1/2$.

Numerical simulations show that for stochastic Hamiltonian systems symplectic schemes produce accurate results for long term simulations [1]. The current work was motivated by the interest to provide a theoretical explanation for the excellent approximations obtained with the symplectic weak scheme (2)-(3).

Firstly, given the solution $\mathbf{X}(T,\mathbf{x}) = (\mathbf{P}(T,p), \mathbf{Q}(T,q))^t$ of the SHS, with $\mathbf{X}(0) = \mathbf{x} = (\mathbf{p},\mathbf{q})^t$, and the corresponding numerical approximation $\bar{\mathbf{X}}_N$ given by the scheme (2)-(3), for any function $f \in C^{\infty}_{pol}(\mathrm{R}^{2n})$, under certain conditions we obtain an expansion of the global error

$$Err(T,h) = E[f(\mathbf{X}(T,\mathbf{x}))] - E[f(\bar{\mathbf{X}}_N)] = -h\int_0^T E[\psi(s,\mathbf{X}(s,\mathbf{x})]ds + O(h^2), \tag{4}$$

for some smooth function $\psi$. Comparing this error expansion and the error expansion obtained in [2] for the Euler scheme, we give a clear justification why the symplectic scheme (2)-(3) produces accurate results while the Euler method produces a very poor solution for the Kubo oscillator, which is a simple linear SHS.

To further investigate the error for the symplectic scheme we do a backward analysis ([3]). The function $u(t,\mathbf{x}) = E(\phi(\mathbf{X}(t,\mathbf{x})))$ satisfies the Kolmogorov equation $\partial_t u(t,\mathbf{x}) = Lu(t,\mathbf{x})$, where L is the order two Kolmogorov operator associated with the SHS, and $\phi \in C^{\infty}_{pol}(\mathrm{R}^{2n})$. Under certain conditions, for any positive integer $M$, we can associate with the first order weak symplectic numerical scheme the modified Kolmogorov operator $L^{(M)}(h) = L + hL_1 + \ldots + h^M L_M$. Based on the approximate solution of the modified flow we obtain an expansion of the error for the numerical solution $\{\bar{\mathbf{X}}_k\}$.

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# Fast Solvers for Models of Incompressible Flow, Linear Elasticity and Poroelasticity and Their Applications in Biomechanics

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Abstract: Fluid flow models, linear elasticity model and poroelasticity model have wide applications in geosciences and biomechanics. For example, blood-vessel wall interactions are modeled by using both fluid flow model and elasticity model; brain edema and cancellous bones are usually modeled by using poroelastic models and the related multiphysics models. In this presentation, I will discuss the Cahouet-Chabard preconditioner using exact and inexact Multigrid solvers for incompressible fluid flow models [1, 2], the two-level overlapping Schwarz methods for linear elasticity model [3, 4], and my recent progress on fast solvers for poroelasticity model [5]. The corresponding applications in biomedical engineering will also be highlighted.

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# Higher order space-time hybridizable and embedded discontinuous Galerkin methods for incompressible flows

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The space-time Discontinuous Galerkin (DG) method is an excellent way to discretize problems on deforming domains. This method uses DG to discretize both in the spatial and temporal direction allowing for an arbitrarily high order approximation in space and time. Furthermore, this method automatically satisfies the geometric conservation law which is essential for accurate solutions on time dependent domains. In this talk, we present higher-order accurate Hybridizable or Embedded Discontinuous Galerkin (HDG or EDG) methods for incompressible flows. The advantage of these methods is that the number of degrees of freedom is significantly less than for a standard DG method. The numerical and scalability tests were carried out using the MFEM library.

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# Modeling the Eddy Currents Induced by the X,Y,Z-Gradient Coils in the MRI Scanner Using the 3D EC-S-FDTD Scheme

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Eddy currents are electromagnetic waves induced by rapidly switching currents of the gradient coils in a MRI scanner. Several finite difference time domain (FDTD) based numerical schemes have been proposed to solve the Maxwell's equations, however many of them have a stability condition. Another numerical scheme, namely, the energy conserved splitting FDTD (EC-S-FDTD) scheme was introduced to solve the Maxwell's equations. It has unconditional numerical stability and conserves the energy property of Maxwell's equations. It has been implemented in the Cartesian co-ordinates for other electromagnetic applications. Typical MRI scanners are cylindrical in shape, hence the use of cylindrical co-ordinates is more numerically efficient. The EC-S-FDTD scheme has been used to model the wave propagation caused by transmission lines and cylindrical waveguides under axial symmetry and also the eddy currents induced by the Z-Gradient coils under azimuthal symmetry. These problems were reduced to 2D cylindrical co-ordinates and produced results similar to the other schemes. The accuracy and efficiency of the 3D EC-S-FDTD scheme should be verified and later applied in various electromagnetic applications. In this paper, we attempt to run numerical simulation in various application in the 3D cylindrical co-ordinates, including approximating the eddy currents induced by the x and y gradient coils of an MRI machine. We will then attempt to use these eddy currents and use the electromagnetic scattering to solve an inverse problem to help distinguish the tissues based on their dielectric properties (electric permittivity and electrical conductivity).

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Title: Numerical Linear Algebra Approach to Cell Image Segmentation

Speaker: Justin Wan, Cheriton School of Computer Science, University of Waterloo

Abstract:

Segmentation of cells in time-lapse bright-field microscopic images is crucial in understanding cell behaviors for medical research. However, the complex nature of the cells, together with poor contrast, broken cell boundaries and the halo artifact, pose nontrivial challenges to this problem. In this talk, we present two robust mathematical models based on linear algebra techniques to segment bright-field cells automatically. These models treat cell image segmentation as a background subtraction problem, which can be formulated as a robust Principal Component Pursuit (PCP) problem which minimizes the rank of the image matrix. Our first segmentation model is formulated as a PCP with nonnegative constraints. In this approach, we exploit the sparse component of the PCP solution for identifying the cell pixels. However, the sparse component and the nonzero entries can scatter all over the image, resulting in a noisy segmentation. The second model is an improvement of the first model by combining PCP with spectral clustering. Spectral clustering makes use of the eigenvectors of the graph Laplacian matrix to classify data. Seemingly unrelated approaches, we combine the two techniques by incorporating normalized-cut in the PCP as a measure for the quality of the segmentation. Experimental results demonstrate that the proposed models are effective in segmenting cells obtained from bright-field images.

**Numerical Methods for Optimal Mass Transport Image Registration**

Yangang Chen, Justin W.L. Wan

We propose a numerical method for solving a non-rigid image registration model based on optimal mass transport. Our main contribution is to address two issues. One is that we impose a proper periodic boundary condition, such that when the reference and template images are related by translation, or a combination of translation and non-rigid deformation, the numerical solution gives the underlying transformation. The other is that we design a numerical scheme that converges to the optimal transformation between the two images. As an additional benefit, our approach can decompose the transformation into translation and non-rigid deformation. Our numerical results show that the numerical solutions yield good-quality transformations for non-rigid image registration problems.

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# Optimization Techniques of Fast Multipole Method (FMM) for Vortex Method Calculation

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In this study, the possibility of acceleration of vortex method calculation has been investigated with the simultaneous use of the FMM [1] and a special purpose hardware, MDGRAPE-3 [2]. Some issues regarding the optimum level of the FMM, and the use of pseudo-particle methods [3] are addressed. Optimization of FMM calculations is an important issue to use it either with or without the use of other techniques such as MDGRAPE-3. The order of multipole moments (here 'p') strongly affects to balance the accuracy and speed of FMM calculation. Higher order multipole moments gives the high accuracy but it requires very high computation cost. On the other hand, lower order multiple moments causes large amount of error while it requires less computation cost.

In this work, the FMM by Cheng et al. [1] has been used. The most time consuming parts of the FMM are the multipole to local (M2L) translation and the direct calculation. The balance between these two steps is dependent on the level of box divisions. Dividing the particles into excessively small boxes will result in an enormous amount of multiple to local tranlations, whereas not dividing them enough would result in a large amount of direct calculation of neighbouring particles. These two steps must be balanced by changing the level of box divisions according to the number of particles being calculated.

At first the various forms of FMM and their performance on MDGRAPE-3 have been considered. The optimization techniques and its performance of the calculation of two colliding vortex rings has been discussed. The collision of two inclined vortex rings at high Reynolds numbers has been simulated in this calculation to check the validity and applicability of proposed method. The dynamics of colliding vortex have been studied and the computation time has been reduced by a factor of 2000 compared to direct calculation on Xeon 5160 (Fig. 1).

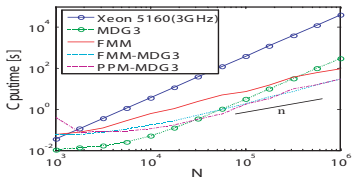


Figure 1: CPU-time of different methods

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# Pruning the Search Trees for Finding the Minkowski Reduced Lattice Bases

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Given a basis for a lattice, the problem of lattice basis reduction is to find a basis for the same lattice consisting of short basis vectors. Lattice basis reduction has a wide range of applications, such as cryptography, signal processing, and geometry of numbers. Among the various notions of lattice basis reduction, Minkowski reduction defines a basis consisting of shortest basis vectors. However, its computational cost is extensive. Inspired by the alpha-beta pruning technique, we propose adaptive search sphere radius and early enforcement of the constraint to reduce the search space for a Minkowski reduced basis. Our experiments show that our techniques can drastically reduce the search time for random data.

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# Time adaptive numerical solution of a highly nonlinear biofilm model in multi-species system with cross-diffusion

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Bacterial biofilms are microbial communities on immersed surfaces, embedded in layers of self-produced extracellular polymeric substances (EPS), which protect the sessile cells against mechanical or chemical washout. Biofilms are prevalent in natural, industrial and hospital settings and available in either beneficial or harmful forms. Mathematical models that help our understanding of the interplay of various biofilm processes reflect the biological complexity of biofilms and are not easy to use. The problem that we consider is a highly degenerate diffusion-reaction model of biofilm formed by multi bacterial species. The model shows three non-linear diffusion effects: (i) porous medium degeneracy which means the density dependent coefficient vanishes as the dependent variable vanishes, (ii) super-diffusion singularity in the density-dependent diffusion coefficient as the dependent variable approaches a known maximum density, (iii) nonlinear cross-diffusion which is a mixture effect of biomass fractions. Biologically relevant solutions are characterized by a moving interface and gradient blow-up there and mixing of species. Due to cross-diffusion effect (iii), the maximum principle does not exist, wherefore simple spatial discretization schemes do not naturally result in systems with M-matrix and non-negativity might not be preserved. We formally treat cross-diffusion as convection and apply a positivity preserving upwinding scheme. Furthermore, our problem at hand has two sources of stiffness. One stems from the disparity of characteristic time scales of substrate diffusion and uptake on one hand, and biomass growth on the other hand. The other one comes into play when the biomass density approaches the super-diffusion singularity. Due to the latter source of stiffness, discretisation of the PDE in space by a standard Finite Volume scheme leads to a singular system of ordinary differential equations. For stiff ordinary differential equations with sufficiently smooth solutions, a host of adaptive numerical methods exists. For our singular ODE system due to the resulting missing regularity of solutions, it is not *a priori* clear whether these can be applied for the time integration of the biofilm equation. Furthermore, it will be important that the resulting numerical scheme is able to deal with sharp biomass gradients at the biofilm/water interface without introducing spurious oscillation or extensive interface smearing. To address these questions, and to propose a fully adaptive method for time integration of the biofilm model is our main objective. We show that singular ODE system has an upper bound solution which is separated from singular point as is required for physical reasons and for agreement with the underlying PDE. This allows the application of error controlled adaptive integration techniques to solve the underlying PDE. The major limitation of existing methods which work with fixed time-steps for solving singular interface moving problems is restriction on time-step size. Error controlled adaptive methods in time can overcome constraints around time integration. Proposed numerical method is validated in a simulation study.

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# Time Second-Order Mass-Preserving Characteristic Schemes and Application to Atmospheric Environmental Computations

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Advection-diffusion process is fundamental in the mathematical modelling of numerous areas of science and technology, such as atmospheric computation, oil reservoir simulation, groundwater modelling, financial modelling. In recent years, it is well recognized that atmospheric aerosols are a great concern for environment and human health. High concentration of aerosols could make severe pollution events, such as urban haze and acid rain, which have significant negative impacts on environment and society. By numerical simulation and prediction of the time evolution of aerosol spatial distributions, aerosol transport models can provide a deeper understanding of aerosol behaviours and are important useful tools for many applications in air quality control and management.

Accurate numerical computation of the advection-diffusion problems is a challenging task, especially for the problems that advection is dominating over diffusion, and for the problems where advective stirring sharpens concentration gradients. The conventional numerical methods often encounter problems of non-physical oscillations and excessive numerical diffusions at steep fronts, while at the same time, these methods can not ensure mass conservation, which is required in various mathematical modelling applications, including atmospheric environmental computation. In atmospheric aerosol transport computation, very small time step sizes usually have to be used by consideration of stability of the numerical schemes used for aerosol advection and diffusion processes, which bring in large computational costs. Therefore, there is a strong interest in developing numerical schemes that permit large time steps and have high accuracy.

In this work, we propose time second-order mass preserving characteristic schemes for advection-diffusion problems. The proposed schemes enable using large time step sizes to get high accurate solutions, while achieves the conservations of variables. Numerical experiments demonstrate the second order temporal and spatial accuracy, as well as mass conservation property by comparing results with exact solutions. Comparisons with standard characteristic finite difference methods show the excellent performance of the schemes that they can get much more stable and accurate solutions and avoid non-physical numerical oscillation. A real case of a severe haze in North China is further simulated and analyzed by using the developed schemes. Simulated results are in good agreement with observations. The developed method can be used for efficiently solving large scale atmospheric aerosol transport problems.

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# Simulating a Mechanical System directly from a Cartesian Coordinate Lagrangian

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For a linkage mechanism—a mechanical system with linked rigid parts and possible other parts such as springs—a Lagrangian approach to the equations of motion is popular because of its economy, and generally leads to a differential-algebraic equation system (DAE) of index 3 or more if cartesian $x, y$ or $x, y, z$ coordinates are used, because of the *rigid-body constraints* involved. High-index DAEs have been seen as hard to solve numerically, so systematic ways have been found to represent the Lagrangian function $L$ in *constraint-free* coordinates, typically angles, leading to an ODE system.

Efficient high-index DAE initial value codes change the balance of advantage. The code DAETS solves a constrained Lagrangian DAE as easily as an ODE. Our recently developed "Lagrangian facility" lets DAETS solve directly from a specification of $L$, purely using algorithmic differentiation—thus without any symbolic manipulation to create the equations of motion explicitly.

We are also developing a "mechanism facility": a way to specify the geometry, kinematics and dynamics of two- and three-dimensional linkage mechanisms, in a tabular form like one that CAD systems often use. From this a cartesian form of $L$ (simple to set up, compared with a rotation-angle form) is derived automatically and solved by DAETS.

We illustrate by examples in 2D (such as the Andrews Squeezer Mechanism, one of the MBS Benchmark problems) and 3D, and report results of numerical solution by this method, with animations.

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# SS-TAVI Theory and Applications of Variational Inequalities

# A hybrid shrinking projection algorithm for fixed point problems and equilibrium problems in Hilbert spaces

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**Abstract:** The purpose of this paper is to address fixed point problems, variational inequality problems and equilibrium problems in the setting of Hilbert spaces. We propose a hybrid shrinking projection algorithm, which exhibits strong convergence in the sense of Mosco, for the construction of a common element in the set of common fixed points of a finite family of nonlinear mappings and the set of common solutions of a finite family of equilibrium problems in Hilbert spaces. Our results generalize and improve various existing results in the current literature.

***2010 Mathematics Subject Classification***: Primary 47H05, 47H09; Secondary 49H05.
***Keywords***: equilibrium problem; variational inequality problem; fixed point problem; nonlinear mapping; inverse strongly monotone mapping; shrinking projection method.

## A New Application of Ostrowski Type Inequality in Engineering

Ather Qayyum

**Abstract:**

Integral inequalities have been extensively researched. However a general theory, that governs the behavior of bounds of Ostrowski type inequalities, has so far not been fully recognized. Integral inequalities are used in innumerable mathematical problems such as approximation theory and spectral analysis, statistical analysis and the theory of distributions. Ostrowski type integral inequalities are one of them, which have a wide range of applications in the field of Engineering. Specifically, it has some very useful applications in numerical analysis. This project is expected to benefit researchers and graduate students working in the fields of integral inequalities, approximation theory, applied mathematics, probability theory and stochastic and numerical analysis.

In this project, improved and generalized version of Ostrowski type integral inequalities will be established for various Lebesgue spaces. The inequalities will be obtained using new and special type of Peano kernels. The use of Peano kernel is the classical approach in establishing different Ostrowski type integral inequalities. Moreover, the parameters used in the Peano kernels help us to recollect previous inequalities which work as a tool for validation of new results. Using these results, new quadrature rules will be established. The establishment of new quadrature rules is one of the major objectives of this project. The proposed research is expected to give quadrature rules which are more efficient both in terms of time consumed and accuracy. Finally, we will attempt to give a particular application for engineering purposes to demonstrate the effectiveness and usefulness of our results.

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# Bifurcations in N-player game dynamics with variational inequalities

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The questions of existence and classification of bifurcation points in a projected dynamics (given by an ODE on a closed convex set arising usually from optimization problems) was studied by various authors so far using either degree theory applied to a variational inequality problem, or using differential inclusions, as introduced by Fillipov. In our most recent work, we encountered equilibrium problems, such as non-cooperative games, where certain parameters induce a change in their associated constrained dynamics; such changes could be appearance or disappearance of periodic cycles, or changes in the number of equilibrium points, or changes in the behaviour of nearby orbits.

While in the classical theory of smooth dynamical systems, these types of changes are clearly studied using mostly the Jacobian of the involved vector field of an ODE, in a constrained dynamics, the non-smoothness of the right hand side poses problems when we are trying to follow the classical approach. We show in this talk that a known mathematical problem called an evolutionary variational inequality (currently used often in time-dependent equilibrium problem formulations) lends itself as a potential straight forward tool in answering the question of existence of bifurcation values for parameters in a constrained dynamics. In this work, we consider the case of a parameter being introduced in both players' payoffs. We denote this parameter by $a \in [\alpha, \beta] \subseteq \mathbf{R}$, where $[\alpha, \beta]$ is a given interval in $\mathbf{R}$. In this case, the equivalent variational inequality problem becomes dependent on the payoffs' parameters. Furthermore, the dynamical system associated to such a VI problem becomes a nonsmooth dynamical system whose right hand side will depend on the payoffs' parameter. Thus we are able to ask the question of whether bifurcations of the associated projected system take place, and what is the meaning of these bifurcations for the initial N-player game.

Last but not least, we give examples of how bifurcation questions can be tackled in this context.

KEY WORDS. Bifurcations, variational inequality, projected dynamical system, N-player games

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# GAME FORMULATIONS FOR DISTINCT CYBERSECURITY INVESTMENT MODELS

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Cybersecurity has become a main focus of investment for retail firms since the dawn of the internet which has revolutionized the way in which most businesses interact with customers and store their information. As the internet has evolved, so has crime, into what we refer to as cyber hacking and cybercrime, and with this cybersecurity was born. In this paper, we model the sellers expected utility subject to constraints, which corresponds to their expected profit.

Expected utility depends on product transactions, investments in cybersecurity, and the buyers preferences. We develop three different games using this model: Nash game, Joint Implementation (Umbrella or generalized Nash) game, and a Cooperative game. In order to find Nash equilibria for these games the KKT systems associated to each scenario are needed; a Nash equilibrium occurs when each seller cannot possibly increase its expected utility without other sellers changing theirs. Given the three KKT systems (one for every game), we compare equilibrium points between games to determine whether one is better than the other. Through analysis of our model, we see that solutions of the umbrella game are also solutions to the Nash game given that the joint constraint function is less than zero. We also observe that Nash solutions can also be solutions to the cooperative game under specific circumstances relating to the profit functions and corresponding item production. Numerical examples are presented to show the different possible outcomes between the three games with varying numbers of firms and buyers. Numerical methods of solving the games rely on variational inequality knowledge and their relation to games.

KEY WORDS. Generalized Nash games, Variational inequality, Projected dynamical system, Cybersecurity investments.

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# On concavity of the monopolist's problem facing consumers with nonlinear price preferences

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A monopolist wishes to maximize her profits by finding an optimal price policy. After she announces a menu of products and prices, each agent $x$ will choose to buy that product $y(x)$ which maximizes his own utility, if positive. The principal's profits are the sum of the net earnings produced by each product sold. These are determined by the costs of production and the distribution of products sold, which in turn are based on the distribution of anonymous agents and the choices they make in response to the principal's price menu. In this talk, we provide a necessary and sufficient condition for the convexity or concavity of the principal's problem, assuming each agent's disutility is a strictly increasing but not necessarily affine (i.e. quasilinear) function of the price paid. Concavity when present, makes the problem more amenable to computational and theoretical analysis; it is key to obtaining uniqueness and stability results for the principal's strategy in particular. Even in the quasilinear case, our analysis goes beyond previous work by addressing convexity as well as concavity, by establishing conditions which are not only sufficient but necessary, and by requiring fewer hypotheses on the agents' preferences.

# VACCINATING POLICY MODELS AS LEADER-FOLLOWER GAMES WITH RISK-PERCEPTION TRANSITION STATES

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Abstract. Vaccination has become an integrated part of public health, since an increase in overall vaccination in a given population contributes to a decline in infectious diseases and mortality. Vaccination also contributes to a lower rate of infection even for nonvaccinators due to herd immunity ([3]). In this work we model human decision-making (with respect to a vaccination program in a single-payer health care provider country) using a leader-follower game framework. We then extend our model to a discrete dynamic game, where time passing is modelled by risk perception changes among population groups considering whether or not to vaccinate. The risk perception changes are encapsulated by probability transition matrices. We consider that the single-payer provider has a given fixed budget which would allow for a potential vaccine coverage of less that 100% of the population. To increase the potential coverage, we introduce a copay policy option, whereby an individual in a largely vaccine inclined population would pay a small portion of the vaccine price. At the other end, we study an incentive policy, where the budget is used to partially entice individuals to vaccinate; we study this policy in a population where the majority of individuals are not vaccine inclined. Last but not least, we allow both policies to be introduced in a population stratified by their risk perceptions as well as by their income.

We see how these policies, together with changes in risk perceptions impact the equilibrium vaccinating decisions of individuals in each group, the potential coverage under budgetary constraints and, ultimately, how it impacts the overall coverage of the vaccine in the entire population. While a copay option on its own seems detrimental to the overall expected vaccine demand, an incentive policy can work to improve vaccine uptake. When further stratified by income, population groups in differing risk perception groups can be subjected to the co-existence of the two policies (copay/incentive) which leads to optimal solutions for both the single-payer provider, and the population's expected vaccine coverage.

**Keywords:** Leader-follower game, Projected dynamics, Copay/incentive policies.

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# Variational inequality theories in reflexive Banach spaces and applications *

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**Abstract**

This presentation is based on recent work on variational inequality theories in reflexive Banach spaces and applications to partial differential inequalities. I'll present the variational inequality theories which are similar to those of fixed point index theories for nonlinear maps, and show how they are applied to tackle the existence of nonzero positive weak solutions of partial differential inequalities with nonlinearities changing signs.

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# Contributed Sessions

# CS-AMPRE Applied Problems and Methods in Research & Education

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# A Time Domain Scheduler for LTE Network and its Performance Evaluation

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The number of users accessing internet through mobile has increased manifold. WiMAX based on IEEE 802.16 and LTE based on 3GPP are two technologies which are used for worldwide access using packet switched architecture. However, LTE has become much popular and widely used technology due to its compatibility with its predecessor technologies such as GSM, CDMA, and WCDMA.
The most promising technology for broadband wireless access with best QoS features for the growing demands of increased number of users and applications is the Long Term Evolution (LTE) mobile system developed by 3GPP[1]. The design of cellular networks is a challenge, as it is required to support tripe play (voice, video and data) service users with varying QoS requirements in terms of throughput, jitter, and delay. An adequate utilization of radio resources is necessary to satisfy QoS requirements of each user and to improve system performance.
In LTE, the task of distributing fixed amount of Physical Resource Blocks (PRBs) among active User Equipments (UEs) every Transmission Time Interval (TTI) is performed by a packet scheduler. The scheduler is located at the MAC layer of evolved NodeB (eNB) e.g. the base station. The downlink LTE scheduler consists of two schedulers: a Time Domain Scheduler (TDS) and a Frequency Domain Scheduler (FDS). The TDS divides the QoS classes into two categories: Guaranteed Bit Rate (GBR) and non-GBR and prioritizes these classes as per their QoS requirements [2]. The FDS follows the TDS and assigns radio resources in terms of frequency. The LTE downlink schedulers are classified as (i) channel unaware schedulers such as RR, WFQ, FIFO, BET (ii) channel aware or QoS unaware such as maximum throughput, PF (iii) channel aware or QoS aware (iv) semi-persistent for VoIP(v) energy aware
The analytical model for LTE scheduler is developed in this paper. However, some extensions and modifications have been applied to the [3] model in order to reflect the LTE context and to provide QoS differentiation among traffic. The performance evaluation using analytical model approximates the behaviour of the system with less time and efforts as compared to experimentation and system simulation. The paper evaluates the time domain scheduler within the LTE network for four applications such VoIP, video streaming, FTP and data. The performance metrics adopted for performance evaluation are throughput and fairness. The voice is mapped to GBR bearer class and video, FTP and data services are mapped non-GBR bearer class. The model is based on the Continuous Time Markov Chain (CTMC).
The results show that the proposed scheduler provides high fairness among applications and satisfies their QoS requirements. The mobile network operators can optimize their radio network and furnish differentiation of services based on their QoS from the analytical model presented in this paper. The analytical model is implemented using *MATLAB*.
Keywords: - LTE, Quality of Service (QoS), Scheduling algorithms, Analytical Model.

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# Applying Data Envelopment Analysis Approach for Measuring Technical Efficiency

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Data Envelopment Analysis (DEA) is employed for measuring the technical efficiency of a sample for libraries of technical colleges. DEA is a non-parametric linear programming based technique used for measuring the relative performance of organizational units where multiple inputs and multiple outputs are present [3]. The main objective of this paper is to provide clear explanation about Data Envelopment Analysis and its step wise mathematical model by using Microsoft Excel solver. The inefficient libraries are identified and the magnitude of inefficiency will be measured. It also investigates how to improve the performance of the inefficient libraries.

Efficiency of a unit refers to its performance in the utilization of resources at its disposal and is a relative concept. It is measured either with respect to the normative desired performance of a unit or with that of any other unit [2]. Technical efficiency means producing maximum output with given inputs; or equivalently, using minimum inputs to produce a given output. DEA is a linear programming based technique for measuring the performance efficiency of organizational units which are termed as Decision Making Units (DMUs). This technique aims to measure how efficiently a DMU uses the resources available to generate a set of outputs [1].

Five libraries of technical colleges are randomly selected for this study, as five different DMUs. One input and two outputs are identified. The input variable is registered readers measured in numbers and output variables are: the number of book collection and staff appointed. Each library is having different numbers of books for their registered readers and it is maintained by their staff.

It was found that three libraries form the efficiency frontier and the other two are inefficient. A benchmark model is recommended for inefficient units. This information can be used to locate the library that require remedial management action and determine the techniques used in efficient library that should be used in inefficient library.

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# ASYMPTOTIC PROPERTIES OF NUMBER OF OBSERVATIONS IN RANDOM REGIONS OF RECORDS

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Let $\{X_n, n \geq 1\}$ be a sequence of independent identically distributed (iid) continuous random variables. Then, the sequences of upper record times, $T_n^U$, and upper records, $X_n^U$, are defined as: $T_1^U = 1$ with probability one, $X_1^U = X$ and for $n \geq 2$, $T_n^U = \min\{j : j > T_{n-1}^U,\ X_j > X_{T_{n-1}^U : T_{n-1}^U}\}$, where $X_{i:m}$ stands for the $i$th order statistic from a random sample of size $m$. Consequently, the upper record-value process is given by $X_n^U = X_{T_n^U}$, for $n \geq 1$. Given a fixed $a > 0$, the random variable $X_j$ is said to be near-record if $X_j \in (X^U(n) - a, X^U(n)]$, and $T_n^U < j < T_{n+1}^U$. Near-record process, which have interesting properties and applicability in insurance theory, were introduced by Balakrishnan et al. [2] and have been studied by several authors, see for example, Gouet et al. [4]. For given $a > 0$, define $\xi_n(a) = \#\{j : T_n^U < j < T_{n+1}^U, X_j \in (X^U(n) - a, X^U(n)]\}, \quad n \geq 1$, as the number of near-records associated to the $n$th record value in a sequence of iid continuous random variables. In this work, we study some properties of $\xi_n(a)$. In fact $\xi_n(a)$ is the number of observations falling in the open left a-vicinity of the $n$th upper record. In the context of order statistics, Akbari et al. [1] obtained some characterization results based on the number of observations near the order statistics. In this paper, we develop the random variable $\xi_n(a)$ by definition a random variable $\xi_n(A)$, the number of observations that fall into a random region determined by a Borel set $A$ that is subsets of positive real number and the $n$th upper record as follows

$$\xi_n(A) = \#\{j : T_n^U < j < T_{n+1}^U,\ \ X^U(n) - X_j \in A\}. \tag{1}$$

In this regard, recently, Dembińska [3] studied the limiting behaviour of numbers of observations that fall into regions determined by order statistics and Borel sets. We investigated the asymptotic behavior of $\xi_n(A)$ in a sequence of iid and absolutely continuous random variables.

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# Feature and Outlier Detection in Magnetograms

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Magnetograms are visual records of moment-to-moment variations in local magnetic fields. Analog magnetogram images were collected at the Agincourt and Toronto geo-magnetic laboratories as early as the 1840s, with records continuing at a variety of observatories to this day. In the 1980s the original photographic paper records were transferred to 35mm film. A recent research project by Natural Resources Canada, and Queen's University has attempted the digitization of these records. With the hope that they could be used for reference, and scientific inquiry.

The records consist of a single sheet of photographic paper, with an example shown in Figure 1. Often these sheets contain two subsequent daily records, a method apparently followed to save on cost. The digitization process begins with scanning these 35mm films, and recording the images in non-glossy format with a resolution of 1964 $\times$ 6236 pixels. The images are then traced using several custom-built algorithms, also attempting to align the series relative to the baselines.

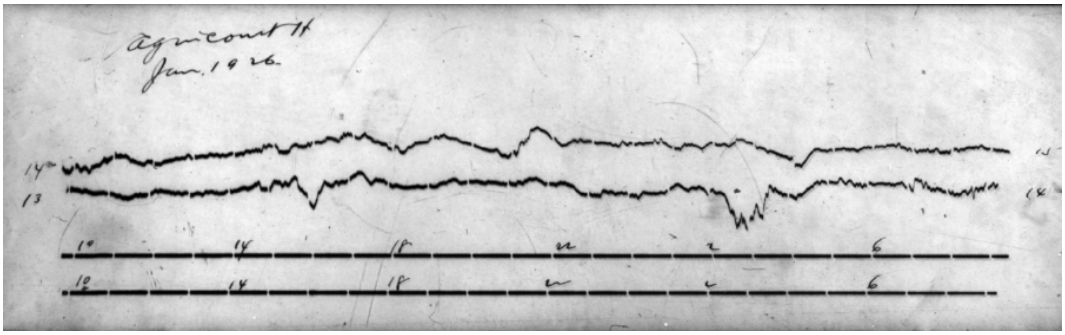


Figure 1: Magnetogram example, recorded at Agincourt on January 13th and 14th, 1926. Notice the timing marks on the recorded baselines.

The steps followed to produce a trace from the digital image are: 1) pre-processing; 2) tracing and pattern detection; 3) trace interpretation; and 4) baseline subtraction and stitching. Each image consists of, at most, 48 hours (in two lines), and the goal is the reconstruction of decades of observations. In step (2), the tracing and pattern detection, the goal is unsupervised or semi-supervised detection of the trace of the magnetic field strength, at the maximum available resolution, from the digital images recorded. In this talk, we will examine several approaches to outlier and feature detection in this context. We will apply an updated data processing pathway to a set of raw images, and discuss the implications for unsupervised processing of the complete ($\sim$ 26,000-element) set of images.

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# Using Social Media to Improve Knowledge Sharing among Healthcare Practitioners

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The number of patients and healthcare practitioners utilizing social media is increasing [1]. Nowadays, social media is considered an interactive channel that can support applications and features that are part of knowledge management systems [2]. As such, social media is a platform is being used to assist healthcare practitioners to enhance the existing skills and knowledge of healthcare practitioners by allowing knowledge to be shared. Typically, healthcare practitioners can easily adapt to computer-mediated collaborative activities and different types of social media and build a 'virtual' social space [3, 4] on a variety of social media platforms, such as Facebook, Twitter, YouTube, online forums and WordPress. Such social spaces, also referred to as online communities of practice, are among the best places for healthcare practitioners to engage in healthcare knowledge sharing because they face the same challenges; share common interests; and engage in similar occupational practices [2-4]. This study discusses the background and increasing importance of using social media for online healthcare knowledge sharing forums and presents a brief literature review. Furthermore, interviews were conducted to gather further in-depth information regarding the experiences of healthcare practitioners in regards to the use of such online forums. The interviewees consisted of one knowledge management academic professor; four healthcare professionals (i.e., a dietician; a laboratory technician; a nurse; and a pharmacist); and one IT technician. Interestingly, the interviewees confirmed the significance of the quality of services and monitoring provided by forum moderators and supervisors. Healthcare practitioners may benefit from participating in healthcare knowledge sharing forums by attaining knowledge that enhances their ability to effectively contribute to issues and dilemmas faced in the healthcare profession; enhancing their problem solving skills and confidence to resolve dilemmas when they arise; becoming familiar with an online community of practice where assistance may be sought concerning problems/issues faced in the workplace; providing access to expertise; and allowing for pleasurable experiences, meaningful participation and a sense of belonging in an online health forums[5, 6].

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# CS-BSM Mathematics and Computation in Biological Sciences and Medicine

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# A Metapopulation Model Incorporating Geographic Mobility Process

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When large numbers of people gather in a limited space for a considerable amount of time, the possibility of spreading infectious disease increases, which can stress the health care system of the host country. It is essential to design strategies to tackle the threat of geographically widespread pandemics. In this study, two mass gatherings and their related outbreaks are analysed: the 2010 Vancouver, BC Olympics measles outbreak and the 2009 H1N1 outbreak connected to the Hajj spiritual gathering in Saudi Arabia. Using SIR models combining both stochastic and deterministic models to study the prevalence of disease among mass migrations, we explain how to incorporate a meta-population model with a mobility process.

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# A Model of Between-Hive Transmission of Nosemosis in an Apiary

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*Nosema ceranae* is a microsporidian parasite of the Western Honeybee (*Apis Mellifera*) that has been implicated in recent Wintering losses of honeybee colonies in regions in Northe America and Europe with colder climates. While the infestation with the disease typically does not lead to failure of a colony, the combined effect of Nosemosis and further stressors can have detrimental effects. In [1], a mathematical model for Nosemosis in a honeybee colony has been presented, consisting of a system of five ordinary differential equations with time-periodic parameters. The dependent variables are healthy and infeced hive worker bees, healthy and infected forager worker bees, and the envrionmental reservoir of spores. Building on this earlier work we develop a mathematical model for the spread of the diseases between hives in an apiary. In this between-hive diseases transmission model each hive in the apiary is presented by the model of [1]. Transfer of the the parasite between hives is assumed to take place in discrete events, for the description of which we follow an approach similar as in [2]. In computer simulation experiments we investigate under which conditions and, if so, how fast the disease spreads in the apiary as a consequence of accidental transfer of spores between hives by the beekeeper during hive maintenance and management operations.

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# A model of highly pathogenic avian influenza in broilers with environmental reservoir and vaccine intervention over finite time

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Avian influenza is a subtype of the influenza A virus which emerged as a highly infectious disease in the 1980's and has caused mass fatalities throughout the poultry industry [1]. Domesticated birds, and specifically broilers, can become infected and spread the disease rapidly due to their genetics and environment. Thus, the addition of interventions such as biosecurity and vaccination are very important in these birds. The objective of this study was to develop a disease model to study highly pathogenic avian influenza in broilers and to analyze the effects of interventions of cleaning and vaccination. An SEIR-type model was developed with the addition of an environmental reservoir to better study the spread of the influenza pathogen. Due to the lifestyle of broilers, the model was studied for a finite time period to predict probable population sizes. The model was then extended to include the addition of an imperfect vaccine. The two models were analyzed for disease free stability and parameter sensitivity.

Economic values play a large role in the poultry industry and have a major influence on decisions. An economic analysis was done to determine the cost effect of an imperfect vaccination versus no intervention. Due to the high variability in avian influenza vaccines and their cost, vaccination is not always the best option. Depending on the efficacy of the vaccine, the size of the population, and the time of culling, vaccination can be worthwhile financially.

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# A Novel Closed-Form Next Generation Operator for Reaction-Diffusion Systems and A Natural Environment For Modeling Movement

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From population range expansion to the spatial spread of infectious disease, reaction-diffusion systems are ubiquitous in mathematical biology. In the context of infectious disease, an important predictive quantity derived from these models is the basic reproduction number. In discrete systems, this number is typically found through the Next Generation Matrix and in the continuum, many operators have been developed as an analog. Here, we examine the limits of the next generation matrix in the continuum to recover the established next generation operators for age-structured models. Applying the same techniques to reaction-diffusion systems leads to a novel closed-form next generation operator. We also make a case for a more natural theoretical environment for the next generation operator in models with more complex movement patterns.

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# An adaptive Magnus expansion method for solving the chemical master equation

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There has been increasing interest in recent years to solve the Chemical Master Equation (CME) directly to analyze the stochasticity of biochemical reacting systems, providing an alternative to popular Monte Carlo methods such as the Stochastic Simulation Algorithm (SSA) or its $\tau$-leaping variants. If the reaction rates are constant, the CME for finding the probability distribution $\mathbf{p}(t)$, given an initial distribution $\mathbf{p}(0) = \mathbf{p}_0$, can be written as an initial value problem

$$\dot{\mathbf{p}}(t) = \mathbf{A} \cdot \mathbf{p}(t), \qquad \mathbf{p}(0) = \mathbf{p}_0. \tag{1}$$

where $\mathbf{A}$ contains the propensities of the reactions with respect to the states, and the theoretical solution is

$$\mathbf{p}(t) = \exp(t \cdot \mathbf{A}) \cdot \mathbf{p}_0. \tag{2}$$

Solving the CME can be a very demanding task due to the large number of possible states in the system, which results in a large matrix $\mathbf{A}$. The Finite State Projection (FSP) [1] truncates the state space and provides a lower bound on the error of the approximation to the true probability distribution. With improvements such as that in the SSA-driven Krylov-FSP algorithm [3], it can be tuned to be even more effective for biochemical systems of reasonable size [2].

However, for many biochemical problems, the reaction rates change over time, making $\mathbf{A}$ time-dependent and so the solution to the CME is no longer (2), and the FSP algorithms that assume $\mathbf{A}$ to be constant cannot be applied. The Magnus expansion [4] provides a way to represent the solution in this case, using

$$\mathbf{p}(t) = \exp(\Omega(t)) \cdot \mathbf{p}_0, \tag{3}$$

where $\Omega(t)$ is an infinite sum whose terms are linear combinations of integrals and nested commutators involving $\mathbf{A}(t)$ at different times. There has therefore been interest to develop numerical solutions to the CME using the Magnus expansion.

We present here a numerical approach with an adaptive state space monitored by SSA [3]. We also explore adaptive time steps based on our analysis of the error. We then compare the results with that of traditional ODE solving techniques such as Adams-Bashforth and Runge-Kutta on two time-dependent biological models [5, 6].

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# Application of Reinforcement Learning in Swarming Problems

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Modeling arbitrary swarm behavior can be a computationally complex problem. In this area, we explore the application of reinforcement learning (using both partial observable and fully observable models) to swarm behavior. This has numerous potential applications ranging from synchronous movement (such as flocking and herding) to search and rescue operations, swarm robotics, and military applications. We devised an approach which can be used for a general swarm problem as well as other applications using this as a generalized methodology. Our results thus far will be described and the key findings will be presented.

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# Communication between viruses influences virulence decisions

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A large class of viruses, the temperate bacteriophages, have two possible life cycles. In the lytic life cycle, the virus infects and kills a host cell, releasing a large number of progeny virus. In the lysogenic life cycle, the virus integrates its genome into the host cell DNA, and two copies of the viral DNA are then produced when the host cell divides. Since lysis confers an immediate fitness advantage, the conditions that may favour lysogeny have been the topic of debate for many years [1]. Recent experimental discoveries have identified viruses that release a short peptide into the environment, a peptide that affects the lysis-lysogeny decision in future generations of the same virus [2]. Here we develop a system of ordinary differential equations to model this novel mechanism of viral communication. The model includes viral populations both in the environment and in bacterial genomes, uninfected and infected bacteria, and the concentration of the communication peptide. By comparison against the same model in the absence of the peptide, we describe conditions under which viral communication confers the greatest advantage, and elucidate parameter regimes that favour lysogeny as a survival strategy for the virus. Stability and bifurcation analysis reveal scenarios in which the ability of the virus to produce the peptide changes the long-term outcome of the viral-bacterial arms race.

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# Comparing the avian and mammalian brain through neural networking

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Avian species have been observed having a very high level of cognition, capable of performing various tasks that many mammalian creatures struggle with [1]. This has long perplexed scientists due to the relatively small size of avian brains. Recently, it has been discovered that avian species have a very high packing density of their neurons [2]. This high packing density causes both shorter axons and higher neuron counts. We investigate the repercussions of this high packing density by using a biological neural network to simulate avian and mammalian neural structures. We simulate various sized avian and mammalian brains (all relatively small) and task them with different problems to observe their behavior. We model these brains as a feed forward neural network with differing delays. Applications of this problem extend to multiple sclerosis research and various agent based tasks such as search and rescue.

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# Conformational change of C6M1 peptide in the presence of salt and lipid: molecular modeling and experimental validation

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Cell penetrating peptides (CPPs) which can cross cell membranes and act as a vector for delivery of biologic molecules have attracted the interest of researchers. C6M1 is a designed CPP which has been used for cellular delivery of short interfering RNA (siRNA). However, the delivery efficacy of the peptide was shown to be affected in the presence of salt, lipid, and other proteins. In this work, the behavior of the peptide in different media with salt and DOPG lipid are investigated using molecular dynamics simulation, circular dichroism (CD), and Fluorescence spectroscopy experiments. We simulated salt and lipid with different concentration ranges of 50 to 300mM and 5 to 15mM, respectively. Furthermore, the experiments were conducted with concentrations varied from 30 to 200mM for salt, and 1 to 40 Molar ratio (MR) for DOPG. The results revealed that by increasing the concentration of salt and lipid, the helical content of the peptide increases significantly about 40-50 percent.

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# Cybernetic Modeling of Growth Dynamics of *Debaryomyces nepalensis NCYC 3413* and Xylitol Production in Batch Reactor

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Growth of *Debaryomyces nepalensis* on mixed substrates in batch culture follows diauxic pattern of completely utilizing glucose during the first exponential growth phase, followed by an intermediate lag phase and a second exponential growth phase consuming xylose. The present study deals with the development of cybernetic mathematical model for prediction of xylitol production and yield. Production of xylitol from xylose in batch fermentation is investigated in the presence of glucose as the co-substrate.

Different ratios of glucose and xylose concentrations are assessed to study the impact of multi substrate on production of xylitol in batch reactors. The concentration of sugars and polyols and enzyme assays were estimated by following the protocol mentioned in the work of Kumar and Gummadi [1]. The model equations for microbial growth, substrate consumption and product formation represented in the present work is way similar to the cybernetic model developed by Kompala and Ramakrishna [2]. The parameters in the model equations were estimated from experimental observations using integral method. The model equations comprising of Ordinary Differential Equations (ODE) and Differential Algebraic Equations (DAE) were solved simultaneously by numerical technique using MATLAB solver. The developed cybernetic model of xylose fermentation in the presence of a co-substrate can provide answers about how the ratio of glucose to xylose influences the yield and rate of production of xylitol.

This model is expected to accurately predict the growth of microorganism on mixed substrate, duration of intermediate lag phase, consumption of substrate, production of xylitol. Cybernetic model of microorganisms best describes the control action of regulatory process when it grows on mixed substrates. The model developed based on cybernetic modelling framework can be helpful to simulate the dynamic competition between the metabolic pathways.

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# Degenerate, diffusion reaction based biofilm growth model on non-orthogonal grids

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Biofilms are a mesoscale collection of bacterial cells growing on wetted interfaces while being held together by an extracellular polymeric network (EPS) produced by the cells. A biofilm growth model which uses a doubly degenerate non-linear diffusion reaction equation for the biomass growth coupled with a semi-linear diffusion-reaction equation for growth limiting nutrients was proposed to model biofilm growth in [1]. The biomass equation includes two interacting non-linear diffusion effects namely porous medium type degeneracy and a super diffusion type degeneracy. The interplay of both effects ensures that the solution of the biomass equation is bounded by the maximum cell density and that spatial expansion of the biofilm only takes place if locally no space is available to produce new biomass.

In all the earlier studies done using the original model as well as its numerous extensions, the biofilm growth has been simulated only in rectangular domains discretized by a 2D orthogonal Cartesian grid with uniform grid spacing used along both the coordinate directions. In this work, to help us simulate the growth of biofilms on rough surfaces which cannot be discretized spatially by an orthogonal grid we extend the formulation to accommodate non-orthogonal grids, i.e., solve equations in non-orthogonal $\xi - \eta$ coordinate system instead of $x - y$. To achieve this end, we modified the semi-implicit method developed in [2] which uses a non-local (in time) representation of the non-linear density dependent biomass flux along with a cell centered finite volume based spatial discretization. In the modified formulation, the biomass flux at the face of the control volume cell is resolved into orthogonal and non-orthogonal components; while the orthogonal component is handled like before, the non-orthogonal component which contains the mixed derivative ($\frac{\partial}{\partial\xi\partial\eta}$) term is handled in an explicit manner and treated as a part of the source term. The validity of the formulation was evaluated by simulating biomass growth in different geometries with and without nutrient transport. In each of these geometries, keeping the initial inoculum same, the biofilm growth was simulated on a sequence of different grids with different degree of non-orthogonality and smoothness. The results from the tests indicate that explicit treatment of the non-orthogonal flux component on the control volume face works as along as the maximum deviation in non-orthogonality ($\theta_{dev}^{max}$) in the region of the grid occupied by biomass is within 20 degrees. With the method established, we simulated the growth of biofilm on sinusoidally rough substratum and investigated the effect the parameters which characterize the roughness (wavelength and amplitude) have on (a) quorum sensing communication between isolated biofilm colonies growing in the adjacent troughs and (b) growth of inoculum layer of uniform thickness at different nutrient concentrations.

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# Dynamics of a Stage-Structured Intraguild Predation Model

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Intraguild predation (IGP), as defined in [4], is killing and eating of potential competitors. An example of IGP is the tri-trophic community module which includes a predator (IG predator) and its prey (IG prey) that share a common resource. Because the IG predator feeds on more than one trophic level, depending solely on both the IG prey and the basal resource for its sustenance, it is a called omnivorous. IGP is a combination of predation and competition. An IGP model of Lotka-Volterra type considered in [1] showed that IGP could have a destabilizing effect, and a criterion for co-existence of all three species is that the IG prey must be superior than the IG predator in competing for the shared basal resource while the IG predator must gain significantly from its consumption of the IG prey. Recently, IGP models [2, 3, 5, 6] are shown to exhibit rich and interesting dynamics such as multi-type bistability and chaos even if the functional responses are linear.

In this talk, we consider a three-species IGP model similar to the stage-structured model examined in [7] but with the IG prey population divided into juvenile and adult stages. The juvenile IG preys are assumed to have little ability of predation and are able to avoid the IG predators by taking refuge. The maturation age of the IG prey population is reflected by a delay parameter $\tau \geq 0$. Conditions for the existence, stability, and bifurcations of all non-negative equilibrium solutions are given using the time delay as parameter. These results are then illustrated using numerical continuation and bifurcation analysis.

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# Estimating Parameters for an Ordinary-Differential-Equation Model Using a Neighborhood Approximation Algorithm

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This paper presents a method for estimating dynamic parameters of a system of non-linear Ordinary Differential Equations (ODEs), which describes the time-dependent dynamics of a marine population. The methodology represents the model parameters with a tessellation of Voronoi cells. It then uses a prescribed rule to generate multiple realizations of the ODE model by selectively sampling specific regions of the parameter space that are characterized by low objective function values. The strength of the methodology, especially in dealing with cases where the ODE model parameters are vaguely known, is demonstrated using synthetic data, as well as real observations.

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# First order systems with functional boundary conditions and their role in applications to medicine and biological models

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In this paper some existence of solution results are presented for the first order coupled system of equations

$$\begin{aligned} u'(t) &= f(t,u(t),v(t)) \\ v'(t) &= f(t,u(t),v(t)) \end{aligned}, \tag{1}$$

with $t \in [a,b]$ and $g, f : [a,b] \times \Re^2 \to \Re$ are $L^1$-Caratheodory functions, subject to the nonlinear functional boundary conditions

$$\begin{aligned} u(a) &= L_1(u(b),v(a),v(b)) \\ u(a) &= L_2(u(a),u(b),v(b)) \end{aligned}, \tag{2}$$

where $L_1, L_2 : \Re^3 \to \Re$ are continuous functions with properties later to be defined.

These functional boundary conditions generalize many of the usual and most common boundary conditions. They are in fact an under used tool in the field of applications. Due to their nature, they can, under the adequate assumptions, be used to study and analyze many applications in diverse areas like biology, medicine, chemistry, engineering, etc.

The methods used are based on the Arzela-Ascoli theorem and Schauder's fixed point theorem, as well as the upper and lower solution method. This analytical method provides direct quantitative and qualitative information not just on the solution, but also on admissible intervals for all the parameters involved.

To emphasize and illustrate these features, two applications are presented and explored. One is an application to the thyroid pituitary homeostatic mechanism and the other is an applications to a nonlinear SIR epidemiological model. In these models, initial conditions exploring this type of functional boundary conditions are introduced, such as global minimum or maximum arguments or integral conditions.

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# Information Transfer-Model Interprets Loss of Control Capability in Biological Systems under External Stimuli

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The loss of variation of state (measured by Shannon entropy) under external stimuli was observed in two biological systems: human myelomonocytic leukaemia cell transcriptional network in response to a phorbol-ester stimulus; soybean metabolic network in response to flooding stimulus [1]. Similar loss of variation of state was suggested in human cellular differentiation [2]. Furthermore, the loss of control capability (robustness) concurrent with the loss of variation of state was suggested [1]. However so far, a mathematical model for the microscopic *Escherichia coli* chemotaxis described the loss of control capability concurrent with loss of Shannon entropy [3].

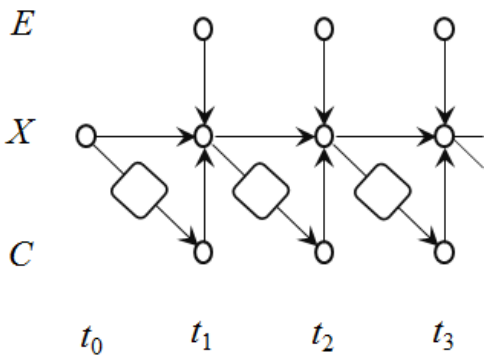


Figure 1: Information transfer model represented by the directed acyclic graph [4].

In this study, we aimed at interpreting the loss of control capability under external stimuli using a mathematical model applicable to general macroscopic systems. We investigated experimental profiles (soybean metabolomic- and human transcriptomic-profiles). They suggested existence of non-linear control elements in the biological systems. We conducted formula analyses based on the information transfer-model including non-linear elements, and interpreted the loss of control capability concurrent with the loss of Shannon entropy under external stimuli (Fig. 1). Furthermore, we validated the results through simulations using ordinary differential equations for a general closed-loop model. In our talk, we will demonstrate the modeling, formulation and simulations. This work was supported by the Japan Society for the Promotion of Science Grants-in-Aid for Scientific Research (grant number: 16K00399).

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# Model Predictive Control of an HBV Model Based on a Nonlinear Kalman Filter

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In this talk, we derive a guideline for efficient drug treatment strategies for hepatitis B virus (HBV) infection. We introduce and analyze a mathematical model that describes the HBV infection during antiviral therapy. The reproduction number $R_0$ is determined. The local/global stability of virus-free steady state is investigated. We formulate a control problem which minimizes the viral load as well as treatment costs. In order to reflect the status of patients not only at the initial time but also at the follow-up visits, we consider the model predictive control based on ensemble Kalman filter and differential evolution. The ensemble Kalman filter is employed to estimate full information of the state from incomplete observation data [1]. We derive piecewise constant drug schedule applying techniques of differential evolution algorithm [2]. Numerical simulations are performed using various weights in the objective functional to suggest optimal treatment strategies in different situations.

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# Modeling the influence of temperature on the sand fly Phlebotomus papatasi's life cycle

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Cutaneous leishmaniasis, a vector-borne disease, classified as a Neglected Tropical Disease, is spread over four continents and it is endemic over 98 countries and territories. Between 0.7 and 1.2 million of new cases are estimated to occur each year worldwide [4]. The disease is transmitted by Phlebotomus species in the Old World and Lutzomyia species in the New World. The incidence of the disease shows a clear dependence on temperature, which varies seasonally [2]. Leishmania parasites that cause the disease proliferate and develop in incriminated vector. Each stage of the life cycle of the vector is influenced by temperature [1]. To address the question on how the temperature affects the disease incidence in Algeria, we developed a structured mathematical model based on Phlebotomus papatasi sand fly life cycle, the proven vector of cutaneous leishmaniasis in Algeria, where entomological parameters were considered to be temperature dependent, to show how the size of the sand fly population varies with temperature. This knowledge could assist decision makers in the choice of appropriate strategies from the available mechanisms, which consists of mechanical control (removing of breeding sites) and chemical control (application of larvicide for larval control and insecticide for adult vector control) at the appropriate time. The derived temperature-dependent basic offspring number, which represents the capacity of vector reproduction, allowed us to assess the impact of the chemical control measures on mortality rates in the larval and pupal stages and adult sand fly over time. Although the mechanical control has no effect on the basic offspring number, it does, however, reduce the total number of breeding sites and, consequently, decreases the carrying capacity.

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# Modelling fitness evolution of HIV-1 including the impact of both viral replication and transmission.

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HIV-1 faces two fitness landscapes: within host where escape from the immune system and competition for host cells drives selection, and between host with the distinct pressures of viral transmission.

Ex-vivo fitness competitions between HIV-1 subtypes have shown subtype C to have a lower replicative fitness than subtypes A, B, and D [1]. In contrast, subtype C has grown to be the dominant subtype globally [1], and our recent meta-analysis has suggested that SHIV subtype C has higher within-host replicative fitness [2].

HIV-1 is a rapidly evolving virus within host, but this rapid evolution is slowed by the presence of the within-host HIV latent reservoirs that lower the replication rate and archive HIV founder strains [4,5]. The HIV latent reservoirs fill early in infection and within the reservoirs the mutation rate is lowered by the error checking of cell division. Between hosts, HIV faces an extreme bottleneck, in that the majority of new sexually transmitted infections are started by a single virus or a single infected cell, ensuring strong transmission selection between hosts [6].

We mathematically model these different evolutionary forces, considering both selection pressure on within-host viral replication and the virus' transmission potential.

Modeling two within-host compartments, an actively replicating compartment with a high mutation rate and a latent compartment with a negligible mutation rate, we investigate the heritability of viral load and transmission fitness. We tune the model with the expectation that any new infection was founded with a low number of virions and demonstrate the role of the latent reservoir in archiving virus from early infection with the goal of reconciling the conflict between ex-vivo and in-vivo results and the effects of selection on the evolution on HIV-1 at the epidemic level.

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# Modelling the spread of Middle East respiratory syndrome coronavirus (MERS-CoV) in Saudi Arabia

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Middle East Respiratory Syndrome Coronavirus (MERS-CoV) has been persistent in the Middle East region since 2012. Abundant scientific evidence showed that dromedary camels are the primary host of the virus. Mathematical modelling of the MERS-CoV camel-to-camel transmission was lacking. In this preliminary work, we first reviewed the temporal patterns of the reported human cases, and then examined several external factors which could affect the transmission of the virus, including the laboratory confirmed influenza A and B cases in six neighboring countries of Saudi Arabia, the timing of Hajj and Ramadan, and climatic factors. Using the plug-and-play likelihood-based inference framework, we fitted a susceptible-exposed-infectious-recovered-susceptible model of camels to the reported human cases with a constant primary-to-secondary human case ratio (i.e. which ranged from one to three) and then estimated a constant spill-over rate. Our results showed that MERS-CoV epidemic waves followed influenza A waves which took off around Hajj, and both transmission were cut off during Ramadan. Longer term surveillance data was needed to test this observation rigorously. For the same reason, we observed no apparent relationships between climatic factors and either influenza or MERS-CoV. Our mathematical model's estimated loss-of-immunity rate and prevalence of MERS-CoV among camels largely matched previous serological or virological studies, shedding light on this issue. By including dromedary camels in animal surveillance and control of MERS-CoV in Saudi Arabia, we could help reduce sporadic introductions to humans.

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# Modelling the suppression of autoimmunity pathogen caused proliferation of T cells

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We study a mathematical model of immune response by T cells where the regulatory T cells (Treg) inhibit interleukine 2 secretion. We model the suppression of the autoimmune line of T cells after a different line of T cells was stimulated by the presence of a pathogen. The exposure to a pathogen results in an increased proliferation rate of the bystander T cells. If the population of the pathogen responding line of T cells becomes large enough, for a sufficiently long time period, it may be able to deplete the concentration of autoimmune T cells. As a consequence, autoimmunity can be suppressed.

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# On the validity of a perturbation flow solution for mass transport calculations in 2D biofilm simulations

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Biofilms are a mesoscale collection of bacterial cells which grow primarily on solid-fluid interfaces by consuming substrate/s from the overlying stagnant or moving fluid while being held together by an extracellular polymeric network (EPS) produced by the cells. A pressure difference driven *"Poiseuille"* flow through a 2D channel with biofilm growing on one or both of the channel walls is a common setup used in the multidimensional, mesoscale biofilm growth studies. These studies require the repeated solution of Navier Stokes equations for the fluid flow and the transport equations for the substrate concentration, calculations which are time consuming and require large grid sizes to resolve the flow features and substrate concentration gradients. Due to these constraints, the studies are often done in narrow channels where biofilm thickness is of the same order of magnitude as the width of the channel. This setup in long term growth simulation studies however suffers from problems arising due to bioclogging. In our current study, we introduce a fast, computationally inexpensive way to compute an approximate flow solution in wider channels using a Boundary Perturbation Method (BPM) and we investigated how the inaccuracies in the flow solution affects the numerical solution of the substrate transport equation calculated using it. The method assumes that the ratio of the amplitude of oscillatory component of the biofilm-fluid interface profile ($A$) to the width of the channel ($H$) given by $\varepsilon = \frac{A}{H}$). It represents the biofilm fluid interface using its finite term fourier series representation and it requires numerical solution of a series of linear ODE's (two for each harmonic in the fourier series representation) which take the form of a two point BVP.

For different biofilm induced channel wall profiles representative of conditions prevalent during biofilm growth, and for a range of flow Reynolds numbers ($Re$) in the channel, on the same refined computational grid we quantified the difference in the steady state substrate concentration solutions computed using an accurate flow solution (obtained from a full Navier-Stokes flow solver) and approximate one obtained using our 1st perturbation order BPM. The results indicate that for representative biofilm profiles considered in the study, the global substrate mass balance, local Sherwood number and substrate concentration along the biofilm-fluid interface as well as the substrate conversion rate computed using these two flow solutions agree well with a few percent for cases where $\varepsilon < 0.1$ and $Re \leq 15$. For values of $Re > 15$ the accuracy of the computed substrate concentration solution calculated using BPM deteriorates. The global conversion rate computed using BPM has a larger value than one obtained using accurate flow solution. This we attribute to large substrate mixing induced by the inaccuracies in the BPM flow solution in the recirculating vortex regions formed downstream of roughness elements present on the biofilm-fluid interface as a result of flow separation. For the range of $(\varepsilon, Re)$ values where it works, the BPM method provides a fast way to compute flow solution which can be used reliably as part of a biofilm growth study.

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# Optimality of asymmetric gears in the legs of a plant-hopping insect

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Optimality principles find wide application in developing a deeper understanding of biological systems; such principles provide a quantitative means by which to account for the complexity observed on a range of biological scales. More specifically, optimality arguments can be exploited to elucidate the possible advantages of morphological adaptations, that is, changes to body shape in animals.

Functional gears have been recently discovered in the ballistic jumping motions of a plant-hopping insect, the nymph stage of the *Issus* [1]. Unlike the most commonly used man-made gears, the gear teeth on the hind legs of the *Issus* are asymmetric. We present an initial investigation addressing the evolutionary question: in what sense are the asymmetric gears found in *Issus* nymphs optimal? Specifically, we investigate the degree to which the differing pressure angles on the drive flank and coast flank are adapted to the loading conditions present during the cocking and propulsive phase of jumping. These questions are addressed through the application of Kapelevich's approach to the analysis of asymmetric gears [2]; in particular the Direct Gear Design methodology offers a technique for maximizing mechanical performance through custom gear design which is well suited to such a reverse engineering application. Optimality of the *Issus* gear parameters is analyzed by examining the gear asymmetry factor and other standard parameters which quantify bending fatigue and contact stress fatigue.

Previous reverse engineering efforts in entomology have lead to the development of new navigational, visual perception, and bionic technologies [3]. Biomemetics in general holds promise of leading to even broader advancements. Thus, a clearer understanding of how evolution has optimized the remarkable structure of the *Issus* gears has wide potential to lead to further innovation.

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# Population dynamics of phages and biofilm bacteria

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Bacteria and their viral predators, bacteriophages, are the most abundant microorganisms on earth. Bacteria have evolved several mechanisms to defend themselves against phages and phages have also evolved to overcome these defence strategies. One of the most important defence mechanisms adopted by bacteria against bacteriophages or any other foreign invader is their group defence, in which bacteria group together in colonies, developing a matrix (extra cellular polymeric substances (EPS)) around themselves. Bacteria are predominantly found in such a biofilm state [1], and biofilm cells are at least 500 times more resistant to antibiotic agents as compared to planktonic (free living) cells [2].

There is a lack of strong evidence of biofilm susceptibility to bacteriophages in nature [3]. Here we develop a four-dimensional ODE model to study the population dynamics of phages and bacteria, where bacteria can be in either biofilm and planktonic states. We approximate this four-dimensional model by a relatively simple three-dimensional model for early-stage biofilm. We also carry out numerical simulations of the early-stage and full models to gain insight into the population dynamics of phages and biofilm bacteria.

Our model can also be considered as a two-patch predator-prey model. In one of the two patches, prey develop a group defence mechanism. To model group defence in a situation, such as the biofilm, in which the population cannot exceed its carrying capacity, we use the simple functional response $f(x) = x(\kappa - \frac{x}{K})$, where $x$ is prey density, $K$ is their carrying capacity and $\kappa$ is a group defence parameter. We show that this function supports the paradox of enrichment.

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# Predictability of Marine Population Trajectories under the Effect of Birth and Harvest Pulses

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That marine populations exhibit complex dynamics, and external influences (i.e. fishing) destroy the system predictability, is known according to [1]. However, this paper adds knowledge to the current by examining, how inter-species delay values, interact with (internal or external) forces, such as birth or harvest events, and how this affects the predictability of the system.

This paper presents the analysis of a single-species and stage-structured Impulsive-Delay-Differential-Equation (IDDE) model, representing a marine population, with focus on understanding

(i) the effect of harvest and birth pulses, and

(ii) the role of delays, in regulating the dynamics of the perturbed system and its predictability.

The paper presents results from numerical experiments. It has been observed that under impulsive events, the system dynamics are predictable for sufficient small delays. However, given large delays, the perturbed system becomes chaotic. At the same time, system disturbances due to stronger impulses were limited, for fixed delays.

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# Spatially-implicit modelling of disease-behavior interactions in the context of non-pharmaceutical interventions

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Pair approximation models have been used to study the spread of infectious diseases in spatially distributed host populations, and to explore disease control strategies such as vaccination and case isolation. Here we introduce a pair approximation model of individual uptake of non-pharmaceutical interventions (NPIs) for an acute self-limiting infection, where susceptible individuals can learn the NPIs either from other susceptible individuals who are already practicing NPIs (“social learning"), or their uptake of NPIs can be stimulated by being neighbours of an infectious person (“exposure learning"). NPIs include individual measures such as hand-washing and respiratory etiquette. Individuals can also drop the habit of using NPIs at a certain rate. We derive a spatially defined expression of the basic reproduction number $R_0$ and we also numerically simulate the model equations. We find that exposure learning is generally more efficient than social learning, since exposure learning generates NPI uptake in the individuals at immediate risk of infection. However, if social learning is pre-emptive, beginning a sufficient amount of time before the epidemic, then it can be more effective than exposure learning. Interestingly, varying the initial number of individuals practicing NPIs does not significantly impact the epidemic final size. Also, if initial source infections are surrounded by protective individuals, there are parameter regimes where increasing the initial number of source infections actually decreases the infection peak (instead of increasing it) and makes it occur sooner. The peak prevalence increases with the rate at which individuals drop the habit of using NPIs, but the response of peak prevalence to changes in the forgetting rate are qualitatively different for the two forms of learning. The pair approximation methodology developed here illustrates how analytical approaches for studying interactions between social processes and disease dynamics in a spatially structured population should be further pursued.

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# The Recurrence-Based Approach for Brain Data Analysis

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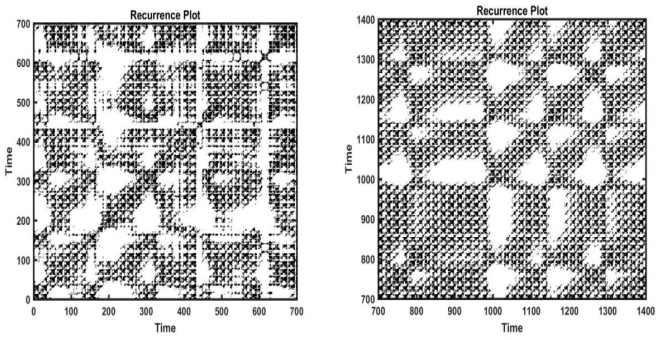
Mathematical modeling and scientific computing play an indispensable role in the development of our understanding of biology. The development of neuroscience has been significantly influenced by modern computational approaches such that many recent remarkable accomplishments have been achieved with the benefit of these techniques.

Recurrence quantification analysis (RQA) is a powerful technique for analyzing nonlinear and complex systems, which includes almost all real-world biological/physiological processes. Notably, the recurrence plot (RP) is an elegant visualization method to display the recurrence points of a dynamical system and perform exploratory data analysis. The intuition of recurrence plots can be traced back to the Poincaré recurrence theorem, demonstrated in the 19th century, whereas the recurrence plot itself wasn't introduced until 1987 by Eckmann et al. [1]. A recurrence plot reveals valuable information regarding the behavior of the system, although it is a very straightforward method to apply.

In this work, we use recurrence plots to study the behavior of intracranial pressure (ICP), the fluid pressure inside the skull, in patients with traumatic brain injuries. Studies show there is a correlation between the ICP and the outcome of patients with brain injuries, suggesting that these signals carry important information about the status of the patient [2]. Our main idea is to find particular patterns in the ICP signals by exploring them with the recurrence plot method. Analyzing the behavior of the system with respect to these patterns could reveal novel insights, such as detecting abrupt changes which may be a sign of change in the patient's status. The hypothesis is that by applying recurrence quantification analysis, we can effectively detect these changes. Our preliminary results suggest distinguishable patterns in these signals which lead us to the next phase of the study: biological and clinical interpretation.




Recurrence plots of multivariate physiological data of a single subject in two different time windows, data from www.physionet.org.

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# Wavelet Coefficient based Fuzzy Inference System for Diagnosis of Malaria

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Malaria is one of the world's most deadly infectious disease leading to morbidity and mortality. In recent times, as a result of climatic changes due to global warming, it is predicted to have unexpected effects on Malaria. In developing countries, visual identification of malarial RBCs may become inefficient due to lack of sufficiently trained technicians and poor-quality microscopes and regents. Thus, new low cost imaging devices and advanced mathematical computing techniques are valuable for determining and distinguishing between the healthy and diseased RBCs.

To choose the right treatment and to ensure a quality of life suitable for a specific patient condition, early and accurate diagnosis of malaria is essential. It will reduce transmission of disease and also prevent deaths. In [1], Anand and et el. used correlation technique on the images obtained from 3-D images produced by digital holographic interferometric microscopy (DHIM) [2], to discriminate the malarial cells from the healthy ones. Our work focuses on designing an efficient, accurate fuzzy inference system [3] for malaria diagnosis based on wavelet coefficients [4].

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# CS-CACO Computational Algebra, Combinatorics and Optimization

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# Authentication Protocol via Zero Knowledge Proof Based on $\alpha$-Skew $\pi$-Armendariz Rings

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A zero knowledge proof is a type of authentication scheme, which gives no knowledge beyond the authenticity for identifying an entity. It is probabilistic more than deterministic authentication scheme. With this type of protocols, many cryptographic operations, such as; authentication, identification, key exchange, etc., are implemented without presenting any secret information through the combination process. The first party must prove knowing the right password without passing any information on that password to the authenticating second party. Ring theory plays an important role in designing of a novel algorithm for zero knowledge proof through using of a particular class of non-commutative rings. In this paper, a new zero knowledge proof based on $\alpha$-skew $\pi$-Armendariz rings is proposed.

The algebraic structure ($\alpha$-skew $\pi$-Armendariz ring) is the heart of this method. Unlike methods raised previously for the zero knowledge proof, our main approach is to build the algebraic structure of the zero knowledge proof depends on the stipulation in the definition of the $\alpha$-skew $\pi$-Armendariz ring. A ring $\Re$ is called $\alpha$-skew $\pi$-Armendariz if for $\varphi(\chi)=\sum_{i=0}^{m}a_i\chi^i, \psi(\chi)=\sum_{j=0}^{n}b_j\chi^j \in \Re[\chi,\alpha]$ such that $\varphi(\chi)\psi(\chi)\in \aleph(\Re[\chi,\alpha])$ then $a_i\alpha^i(b_j)\in \aleph(\Re)$ for each $i$, $j$ [1]. Here, $\Re[\chi,\alpha]$ represents the polynomial ring in $\chi$ with respect to an endomorphism $\alpha$ of $\Re$, such that $\chi r=\alpha(r)\chi$, where $a_i$, $b_j$ and $r\in\Re$. Also, $\aleph(\Re)$ is the set of all nilpotent elements of $\Re$. The concept of $\alpha$-skew $\pi$-Armendariz rings is defined motivated by the notions of $\alpha$-skew Armendariz rings [2] and $\pi$-Armendariz rings [3].

The proposed method used a secret polynomial whose coefficients are in an $\alpha$-skew $\pi$-Armendariz ring. This polynomial is kept by the prover, the algebraic structure of the proposed zero knowledge protocol does not reveal any information about the secret polynomial. It is well known that many cryptographic systems can be constructed based on polynomials and functions over finite fields. The statements that will be concerned in this paper are of the form $\varphi(\chi)\in\Re[\chi,\alpha]$, where $\Re$ is an $\alpha$-skew $\pi$-Armendariz ring. For $\varphi(\chi)=\sum_{i=0}^{m}a_i\chi^i, \psi(\chi)=\sum_{j=0}^{n}b_j\chi^j\in\Re[\chi,\alpha]$, we consider $\varphi(\chi)$ is the secret polynomial, and the prover wants to convince the verifier that $a_i\alpha^i(b_j)\in\aleph(\Re)$ without revealing anything else about $\varphi(\chi)$. In particular, the prover does not reveal the polynomial $\varphi(\chi)$. The properties of the $\alpha$-skew $\pi$-Armendariz zero knowledge proof is investigated in terms of: 1- Completeness: The authorized prover can always convince the verifier, 2- Soundness: The authorized prover cannot convince the verifier with some rate called "soundness error" (even if the prover cheats and deviates from the protocol), 3- Zero knowledgeness: The verifier cannot know anything from the protocol and cannot claim to be the prover to any third entity and the prover cannot deceive the verifier. Hence, the verifier does not learn anything except the fact that the statement is true. We found that, the proposed protocol satisfies the completeness, the soundness in the sense that, there is 50% chance of catching a cheating prover, and the proposed protocol has the property of zero knowledge.

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# Exact Coloring of Sparse Matrices

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Given the sparsity pattern (location of nonzero entries) of a matrix $A \in \mathbb{R}^{m\times n}$ we consider partitioning $A$'s columns into groups with the property that no two columns in the same group have nonzero entries in the same row position. Formally, let $\Phi$ be a mapping defined as $\Phi : \{1,2,\ldots,n\} \mapsto \{1,2,\ldots,p\}$ such that $\Phi(j) = \Phi(l), j \neq l \Rightarrow \nexists i$ for which $a_{ij} \neq 0$ and $a_{il} \neq 0$. In other words, each column receives a color (group) label from the set $\{1,2,\ldots,p\}$ such that the columns receiving the same color label satisfy the property that they are "structurally orthogonal" [1]. The problem we want to solve is to find a mapping which minimizes the number of groups or colors $p$. This problem and its many variants arise in computational optimization where first- and higher-order derivatives (gradients, Jacobians, Hessians) of some differentiable function need to be evaluated in an iterative scheme e.g., in Newton's method and is known to be NP-hard [2, 5]. A vast majority of research on the matrix coloring problem are concentrated around developing efficient heuristic techniques.

In this paper, we study exact coloring methods based on implicit enumeration. The coloring problem that we consider has useful structures that can be exploited when formulated and implemented as a matrix coloring problem. A widely used enumeration exact coloring code first finds a maximal clique, assigns colors to its vertices, and then performs a branch-and-bound type search with back-track [6]. The graph is represented by its adjacency matrix. In the matrix coloring problem, however, each row $i$ for $i = 1,2,\ldots,m$ the columns $\{j|a_{ij} \neq 0\}$ are mutually structurally dependent and therefore defines a clique in graph-theoretic sense. Thus a maximal clique is obtained by identifying a row with the maximum number of nonzero entries. In our computer implementation, we employ compressed sparse data structures to represent the sparsity pattern of the matrix. Additionally, we utilize a bucket data structure to choose the next vertex to be colored [4]. We explore several chromatic degree-based vertex selection approaches and alternative tie-breaking strategy. Our exact coloring implementation can be used independently or as a subroutine to color a small critical submatrix in a combined approach where the partial coloring is extended to the entire matrix using heuristics [3].

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# Investigating Optimization Parameters for an Evolutionary Algorithm

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Evolutionary algorithms can be used as a mechanism to solve complicated problems in optimization [1, 2]. In the schemes that we are concerned with, we consider a pool of *individuals*, defined by a set of parameters, that are defined in a first *generation*. Each individual is a potential solution to a problem; for example, we may have a desired goal of optimizing a particular function. In every generation, each individual in the pool serves as input, while the output determines the *fitness* of each individual. Then, at the conclusion of each generation, results from each individual are compared, and a *selection phase* occurs. This selection phase reduces the number of individuals in the pool according to their fitness in some way, either deterministically (by specifying the individuals) or according to some probability (through the use of a *survival function*); the method of selection may even be chosen to adapt over many generations [3]. Then, to begin the next generation, a new pool of individuals are developed based on those that were selected from the previous generation, with a small possibility of *mutations* being introduced to each individual, expanding the variety of solutions that could be considered. This process increases the average fitness of individuals and is repeated until some particular criteria is met.

Individuals representing creatures and movement have been explored as an application of evolutionary computation [4]. We detail a specific direct problem of this sort: Consider individuals that consist of collections of *nodes*, *muscles*, and *bones*, defined as components of three-dimensional geometric shapes. The goal is to optimize forward movement in a three-dimensional environment within a given time, and this goal determines the fitness of each individual. Different considerations, parameter choices, possible mutations, selection methods, and trends of fitness over the generations given these choices will be discussed. Then, we consider an inverse problem: Given a desired level of fitness, on average, within a generation pool, what selection methods or parameter choices will achieve this in the smallest number of generations? The chance of mutation at each generation and the choice of selection methods will be discussed.

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# Topological Indices on Different Networks

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*Topological index* or *Molecular descriptor* is obtained by transforming the chemical information into a numerical number. Topological index is a molecular graphics invariant which is the correlation with the physico-chemical properties of a molecular graphical numbers. There are three important types of topological indices like Distance based topological index, Degree based topological index and Counting related polynomials index of the graphs. In 1947, Harry Wiener[8] introduced the *wiener index*. His success based on it, chemical graphs have many other topological indices consist of information of molecular branching[7].

After Wiener's work index another, a freshly introduction of *Szeged index* [2], which is same kind of winner's denoted by $S_z$ is a newly introduced in graph invariant and a certain types of chemical applications were reported in mentioned references[4,5,6].

In 1972, *Zägreb* indices have been introduced by *Zägreb* Group by Ivan *Gutmán* and *Trinájstić*[1]. Second Zagreb index was think of by *Gutmán* et al. in 1975 [3].
In this paper, we will compute the degree based topological indices the so-called general *Randić* index $R_\gamma(G)$ for $\gamma = \{1, \frac{1}{2}, -1, -\frac{1}{2}\}$, atom bond connectivity(ABC), geometric-arithmetic(GA), first*zägreb*, second *zägreb*, second modified *zägreb*, third *zägreb*, hyper *zägreb* and augmented *zägreb* topological indices for subdivision of different kinds of networks like silicate sheet, chain silicate network, Hexagonal, Honeycomb, Butterfly and Benes networks as well as molecular structural networks. This study will give us a very interesting and different results by using above topological indices.

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# Unitary operator decompositions applied to quantum circuits

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Quantum physics offers a new paradigm in which the laws of quantum mechanics are used to design algorithms that can surpass a classical computer. Quantum computation has been of growing interest since the mid-1990s with the discovery of a quantum algorithm allowing efficient factorization of integers. This algorithm, described by Shor [1], can quickly break most of the traditional means of encryption such as RSA.

In quantum computation, the state of a n-bits register is not a binary state anymore but a state vector $|\psi\rangle$ which is a normalized complex linear superposition of all the possible binary states :

$$|\psi\rangle = \sum_{b\in\{0,1\}^n} a_b |b\rangle\,, \text{ and } \sum_{b\in\{0,1\}^n} |a_b|^2 = 1. \tag{1}$$

The state evolves by unitary transformations and the synthesis of such transformations into a quantum circuit - the quantum equivalent of a logical classical circuit - is of particular interest. Given a library of elementary quantum gates and some architectural constraints, it is crucial to be able to find, if possible, a circuit that can implement the unitary operator efficiently i.e with polynomial size or depth.

Most methods today use different factorizations of unitary operators (e.g., Cosine-Sine and Block-ZXZ decompositions [2, 3]) but very few of them try to exploit auxiliary qubits in order to reach new decompositions. The reuse method, using extra memory to synthesize linear combination of efficient subcircuits, is one of them [4]. In this context we propose a deep overview and improvements of some of these methods. We compare them according to different criteria (complexity, set of gates, memory, architecture) and give some insight about their industrial interest. Especially, attention will be given to ways of using numerical optimization methods, running on High Performance Computers, in order to deal with problems of non-trivial size.

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# CS-CPC Computational Physics and Chemistry

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# A DG Method For Neutron Transport Equations on 3-D Unstructured Grids[1]

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Time-dependent neutron transport equation is a kind of important hyperbolic partial differential equation in nuclear science and engineering applications. High dimension neutron transport calculation include computing of space grid, angle direction, energy group and time step, is very complex and huge scale scientific calculation problem. Discontinuous finite element discrete ordinates (DFE-Sn) method is very efficient for solution of such equations especially while concerned with complicated physics including multimedia, larger grid distortion, complex initial and boundary conditions.

In this paper, the discrete scheme of Sn discrete ordinate and discontinuous finite method 3-D unstructured tetrahedral meshes are presented. We developed a serial solver with DFE-Sn method to solve time-dependent neutron transport equations on unstructured tetrahedral grids. Domain decomposition scheme, parallel Sn sweep algorithm and multi-level Parallel Algorithm on unstructured grids are adopted to improve the efficiency, the parallel computation for the scheme is realized on MPI systems. Numerical experiments demonstrate the accuracy and efficiency of these methods.

**Key words:** DG method, transport equations, unstructured meshes, domain decomposition, sweep algorithm

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# A Higher Order Space-Time Numerical Method for Compressible Flows

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We present a highly accurate numerical method based on the Spectral Deferred Corrections (SDC) time integration technique and the Essentially Non-Oscillatory (ENO) finite volume method for the compressible fluid flow applications. The SDC technique is used to advance the solutions in time with high-order of accuracy. The ENO method is used to calculate numerical fluxes with non-oscillatory fashion. The coupling of the SDC method with a high-order finite volume method (Piece-wise Parabolic Method (PPM)) for solving the conservation laws is first carried out by Layton et. al. in [1]. Kadioglu et. al. [2] have addressed issues about this approach and introduced some improvements. Here, we investigate the implications when the PPM method is replaced with the well-known ENO method. We note that the SDC-PPM method is fourth-order accurate in time and space. We kept the order of accuracy of the ENO procedure as fourth-order in order to be able to make a consistent comparison between the two approaches (SDC-ENO versus SDC-PPM methods), otherwise in theory the ENO procedure can be arbitrarily higher order. We have tested the new SDC-ENO technique by solving several test problems involving moderate to strong shock waves and smooth/complex flow structures [3]. Our numerical results show that we have numerically achieved the formally fourth-order convergence of the new method for smooth problems. Our numerical results also indicate that the newly proposed technique performs very well providing highly resolved shock discontinuities and fairly good contact solutions. More importantly, the discontinuities in the flow test problems are captured with essentially no-oscillations. We have numerically compared the fourth-order SDC-ENO scheme to the fourth-order SDC-PPM method for the same test problems. The results are similar for most of the tests except in some cases the SDC-PPM method suffers from minor oscillations compared to SDC-ENO scheme being completely oscillation free.

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# A Path Integral Hybrid Molecular Dynamics Approach to Investigate Rotations and Bosonic Exchange at Low Temperature

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Traditionally, the Hamiltonian in Path Integral Molecular Dynamics (PIMD) codes include solely the kinetic and potential energy operators, which can sufficiently describe properties of many quantum systems. However, for rigid rotor systems in which the Hamiltonian requires the rotational kinetic energy operator, bosonic systems in which the partition function requires permutations of the positions of identical particles, or systems containing both, traditional PIMD will not suffice and Path Integral Monte Carlo (PIMC) [1] must be used. This is because it is extremely difficult to introduce the equations of motion of the rigid body rotations into PIMD and the main methods to sample bosonic exchange are solely Monte Carlo-type algorithms.

We propose a hybrid code, where molecular dynamics is used for the translational motion of the particles (using the Langevin equation thermostat [2]) and Monte Carlo is used for both the rotations of the rigid rotor[3] and the nuclear exchange of bosonic particles (called the WORM algorithm [4]). This WORM algorithm is the first implementation in a molecular dynamics framework and by including this nuclear exchange, the superfluid fraction of helium or hydrogen clusters surrounding a dopant molecule can be calculated as a function of temperature and cluster size. Although hybrid codes exist, for example Path Integral Hybrid Monte Carlo [5], we accept all of our molecular dynamics translation steps and sample our rotations/exchanges separately.

One study [6] which demonstrates the importance of rotations and exchange involves the vibrational shift of a $CO_2$ molecule (rigid rotor) placed in a cluster of $N$ bosonic helium atoms. The shift was calculated with traditional PIMD, PIMC without exchange or rotation, PIMC with exchange, and PIMC with exchange and rotation and the results were compared to experiment. The only curve that agreed with experiment was PIMC with exchange and rotation. We investigate clusters of HF to test our rotation code and $pH_2$ to test our WORM algorithm with a goal to reproduce the $CO_2 - He_N$ experimental results with our hybrid PIMD framework.

A main advantage of PIMD is it's extension to Ring Polymer Molecular Dynamics (RPMD) [7], which allows for the calculation of approximate real-time dynamic properties through correlation functions, of which PIMC has no analog. The ability to calculate approximate real-time dynamics of systems including rotation and nuclear exchange would be extremely beneficial to the scientific community.

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# Cell selectivity of peptide antibiotics: an experimental illusion or peptide intrinsic quality?

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The excessive use of conventional antibiotics has raised a serious problem known as antibiotic-residence of bacteria. Naturally-occurring antibiotics, i.e., antimicrobial peptides (AMPs), have been used as templates for developing new therapeutic agents. Good AMPs should be able to discriminate between host and bacterial cells. The "quality" of AMPs is often measured by their cell selectivity. Despite its significance, however, the selectivity has not been systematically examined. As a result, it has often been overestimated. Here, we present a coarse-grained model of peptide selectivity, especially one that shows how cell densities ($C_{\text{cell}}$) are implicated in the selectivity, resolving earlier confusions about the selectivity. Using the model, we relate peptide's intrinsic ($C_{\text{cell}}$-independent) quality to an apparent, $C_{\text{cell}}$-dependent one, and establish peptide-parameter-activity relationships. This effort will benefit our endeavour in optimizing the peptide parameters for their enhanced selectivity.

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# Combining Deflation and Nested Iteration for Computing Multiple Liquid Crystal Equilibrium States

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Multiple equilibrium states arise in many physical systems, including various types of liquid crystal structures. Having the ability to reliably and efficiently compute such states enables more accurate physical analysis and understanding of experimental behavior. In this talk, we consider adapting and extending a deflation technique for the computation of multiple distinct solutions arising in the context of modeling equilibrium configurations of nematic and cholesteric liquid crystals. The deflation method is applied as part of an overall free-energy variational approach and is modified to fit the framework of optimization of a functional with pointwise constraints. The system is highly nonlinear and, under certain conditions, generates many distinct equilibrium states. It is shown that multigrid methods designed for the undeflated systems may be applied to efficiently solve the discretized linear systems arising in the application of deflation. For the numerical algorithm, the deflation approach is interwoven with nested iteration, creating a dynamic and efficient method that further enables the discovery of distinct solutions. Finally, we present numerical simulations demonstrating the efficacy and accuracy of the algorithm in detecting important physical phenomena, including bifurcations and disclination behaviors.

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# Thermodynamic Properties of Nonadiabatic Systems

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The goal is to obtain thermodynamic properties, specifically the Gibbs free energy $G$, of nonadiabatic systems. Nonadiabatic systems are of importance in numerous fields such as photo-chemistry, biology, quantum information processing, and electro-chemistry. Efficient calculation of $G$ and $\Delta G$ enables high-throughput screening for catalytic materials. [1, 2]

Only nonadiabatic systems that can be described by a vibronic Hamiltonian, obtained through electronic structure calculations, are investigated. A Path Integral Monte Carlo (PIMC) approach is used to calculate thermodynamic properties from these precalculated vibronic Hamiltonians. Hamiltonians are evaluated in a product basis of nuclear and electronic degrees of freedom. The resolution of the identity for this space can be expressed as

$$\boldsymbol{I} = \int \mathrm{d}\mathbf{R} \sum_{n=1}^{N} |\mathbf{R}, n\rangle \langle \mathbf{R}, n| , \tag{1}$$

where $\mathbf{R}$ is a vector of length $f$ representing the nuclear positions, and $n$ indicates electronic surfaces. The partitioning of the Hamiltonian operator into a harmonic oscillator operator and a coupling operator is a key step in our methodology:

$$\hat{H} = \hat{h}_{\mathrm{o}} + \hat{V}. \tag{2}$$

Using this form of the Hamiltonian, the partition function of the full system can be expressed as the product of an expectation value and the partition function of $\hat{h}_{\mathrm{o}}$:

$$Z_{\mathrm{H}} = \Big\langle g(\mathbf{R}) \Big\rangle_{\varrho} \Big( Z_{\mathrm{ho}} \Big). \tag{3}$$

The advantage of this formulation is computational efficiency. The $Z_{\mathrm{ho}}$ can be calculated analytically. Calculating the expectation value is efficient because samples are drawn without rejection.

Preliminary results indicate that we are able to obtain the partition function and internal energy of model systems. The Gibbs free energy can be obtained through the thermodynamic relation

$$G = pV - k_B T \ln(Z). \tag{4}$$

In the future we aim to accelerate the calculations for larger systems with the use of graphics processing units (GPU's).

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# CS-DSDE Applications of Dynamical Systems and Differential Equations

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# A new approach to construct first integrals and closed-form solutions of dynamical systems for epidemics

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The dynamic optimization problems arise in mechanics, physics, biology, economic growth theory, engineering and many other fields of applied mathematics. The three fundamental techniques to solve the dynamic optimization problems are calculus of variation, dynamic programming and optimal control theory. The optimal control theory developed by Pontrygin [1] utilizes a Hamiltonian function. The standard and non-standard Hamiltonian functions are real physical structures. The canonical Hamiltonian system $\dot{q}^i = \frac{\partial H}{\partial p_i}, \dot{p}^i = -\frac{\partial H}{\partial q_i}$ arises for a standard Hamiltonian. The non-standard Hamiltonian system $\dot{q}^i = \frac{\partial H}{\partial p_i}, \dot{p}^i = -\frac{\partial H}{\partial q_i} + \Gamma^i(t, q^i, p_i)$ appears for the non-standard Hamiltonian. A new class of non-standard Hamiltonian known as the "artificial Hamiltonian" is introduced which results in an artificial Hamiltonian system of first-order ordinary differential equations (ODEs). The notion of an artificial Hamiltonian is developed for the systems of dynamical systems of ODEs. Also, it is shown that every system of second-order ODEs can be expressed as an artificial Hamiltonian system of first-order ODEs. The newly developed notion of an artificial Hamiltonian system gives a new way to solve the dynamical systems of first-order ODEs or systems of second-order ODEs which can be expressed as an artificial Hamiltonian system by utilizing the known techniques applicable to the non-standard Hamiltonian systems. We employed this proposed notion to solve dynamical systems of first-order ODEs arising in epidemics.

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# Comparison of Closed-form Solutions for the Lucas-Uzawa model via the Partial Hamiltonian Approach and the Classical Approach

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In this paper we establish the closed-form solutions for the Lucas-Uzawa model with the aid of the partial Hamiltonian approach and we compare our results with those derived by the classical approach. The partial Hamiltonian approach provides two first integrals [1] for case where there are no parameter restrictions. We utilize these two first integrals to construct closed form solutions for all variables of model for two different scenarios: (i) $z = z^*$ and (ii) $z \neq z^*$ where $z(t) = \frac{h(t)u(t)}{k(t)}$ where $k(t)$ is physical capital, $h(t)$ is human capital and $u(t)$ is the fraction of labor devoted to the production of physical capital. We begin by using both first integrals to construct closed-form solutions for both scenarios. One solution is exactly the same as derived by Chilarescu [2] and the second is completely new to the literature. We then use only one first integral to determine a different solution, again under fairly general parameter values, and show that this is the same solution that has been derived in the previous literature (see [2]). We find that in the case where $z = z^*$, both the partial Hamiltonian approach and the classical approach provide one solution. For the $z \neq z^*$ case, the classical approach yields one solution while the partial Hamiltonian approach yields the same solution as well as providing one additional solution which is completely new to the economic growth literature. What is especially interesting about our new solution is that while the equilibrium levels of consumption and capital stock in the new solution are equal to those found in the old solution, the amount of labor allocated to the production of physical capital and the level of human capital are different in the new solution. In the context of economic growth theory, this means that an economy can be in either a high or low human capital equilibrium. The existence of three closed form solutions is new to the literature and we also show that these closed form solutions all converge to the same long run balanced growth path.

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# Computation of the expansion of Melnikov functions around a homoclinic loop

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In this talk, we study homoclinic bifurcation of limit cycles in perturbed planar Hamiltonian systems given by

$$\dot{x} = H_y + \varepsilon f(x,y,a), \quad \dot{y} = -H_x + \varepsilon g(x,y,a), \tag{1}$$

where $H$, $f$ and $g$ are analytic functions on the plane $\mathrm{R}^2$, $a \in \mathrm{R}^m$ is a vector parameter, and $\varepsilon \in \mathrm{R}$ is small. The number of limit cycles in system (1) bifurcating from the family of periodic orbits $L_h$ defined by $H = h$ can be estemated by isolated zeros of Melnikov function

$$M(h,a) = \oint_{L_h} g\mathrm{d}x - f\mathrm{d}y.$$

Suppose that a homoclinic loop $L_{h_s}$ is defined by $H = h_s$, and $L_{h_s}$ is the outer boundary of periodic orbits $L_h$ for $h < h_s$. From [1, 2] the expansion of $M(h,a)$ near $h = h_s$ is

$$M(h,a) = \sum_{j\geq 0} [c_{2j}(a) + c_{2j+1}(a)(h-h_s)\ln|h-h_s|](h-h_s)^j. \tag{2}$$

There are very few results about the computation of the coefficients $c_j$. Only the first four coefficients $c_j$ have been obtained in [3, 4]. Our main result is that a new method is established for computing the coefficients $c_j$ in (2). Then by using those coefficients, more limit cycles would be found around homoclinic loops. An example is also provided to illustrate our method.

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# Coupled Axial, In Plane and Out of Plane Bending Vibrations of Cable Harness Space Structures

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This paper presents a distributed parameter model to study the effect of cable harness on the space structures. We assume the space structure behaves like a Euler-Bernoulli beam. A straight cable (see Fig. 1) is attached along the length of a rectangular beam. Existing continuum models assume various vibration degrees of freedom (DOF) such as bending, axial etc. are decoupled [1]. We position the cable at an offset distance along the y-axis. As a result, the system will have significant amount of coupling between the axial, in plane bending and out of plane bending DOFs. The main goal of this paper is to highlight the importance of using a coupled vibration model to estimate the eigenfrequencies of a cable harnessed structure.

Extended Hamilton's principle is used to develop the governing coupled partial differential equations (PDEs) of the cable harness beam. The eigenfrequencies and eigenfunctions for the coupled PDEs are found out using analytical method [2]. The eigenfrequencies obtained from the coupled and decoupled PDEs will be compared to the results obtained from the Finite Element Analysis (FEA) formulation. The same analysis will be repeated by varying cable parameters such as the radius, offset position and the young's modulus.

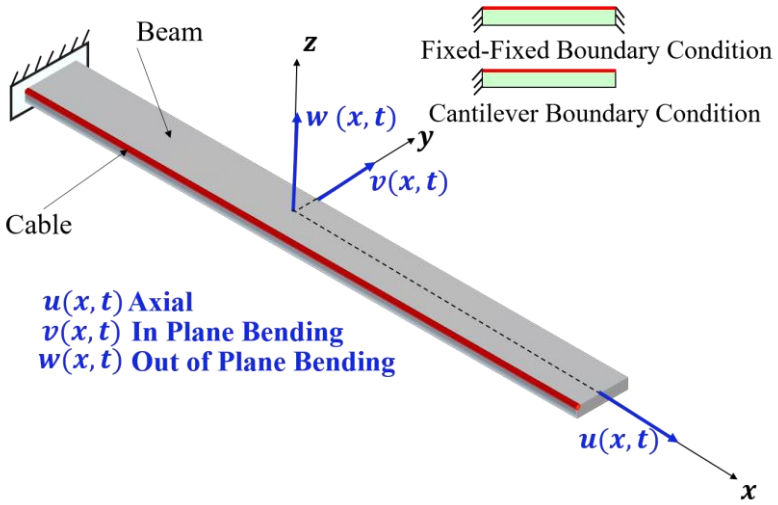


**Fig. 1** Representation of the cable harness beam along with the coordinate axes. $u, v, w$ represent the vibrations in the axial, in plane bending, out of plane bending direction respectively.

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# Dynamical analysis of a modified predator-prey model for Venture Capital Investment

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The Lotka-Volterra [1, 2] predator-prey model, which proposed the population dynamics between predator and prey species, has been an important model in Biology for many years. It consists of a pair of first-order, non-linear differential equations which describes the interaction of the two species. It has been subsequently applied to different fields such as Ecology, Chemistry, Mathematics, Business, Economics and Finance. Most recently, Brander and de Bettignies [3], considered the use of a predator-prey model to explain the relationship between Venture Capital investment opportunities and the experience of the investors, which represent the prey and predator respectively. Our work extends this model to include a modification with two investment opportunities available to the venture capitalist. Stability analysis is performed using slight perturbation around the non-zero, interior equilibrium point to determine where the system loses stability. The dynamics of the system are investigated via analytical work and numerical simulations. Results are presented numerically and graphically. It is seen that the variation of certain parameters causes the system to experience bifurcations and the stability changes. This model attempts to provide a guide, using the stability regions for various parameters, to determine whether or not mathematics can be used to explain if the venture capitalist should make the investment or not.

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# Exact Solutions of the Equations of Motion of a System of Two Coupled Lagrange Tops in a Central Gravitational Field

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The subject of rigid body dynamics is two and half centuries old. It is dated back to L. Euler who derived the now classical equations of motion of a heavy rigid body about a fixed point and solved them in the case when the moment of external forces acting on the body is equal to zero. It was a first exact solution in multibody dynamics. Since then this problem and its various generalizations have attracted the attention of many prominent scientists (see [1, 2, 3] and references therein). In particular, a great deal of work [1, 2, 4, 5] has been devoted to studying the properties of the equations describing the dynamics of a rigid body in a central gravitational field.

Compared with the equations of motion of a single rigid body, the analytical study of mathematical models for a system of hinge-connected rigid bodies is a much more complicated problem [4, 6]. As a consequence, there are very few known cases of integrability in the dynamics of many-body systems [4, 6, 7, 8].

In this paper we study dynamical properties of a system of two coupled Lagrange tops moving about a fixed point in a central gravitational field. We construct a new class of exact solutions of the equations governing the system's motion. The new solutions describe the motion of the multibody system with the following property: the tops' dynamic symmetry axes belong to a vertical plane rotating about the vertical line passing through the system's fixed point while at the same time the axes change their position relative to the plane in a similar fashion. We establish conditions on the multibody system's parameters guaranteeing the existence of the new solutions and conduct the compatibility analysis of these conditions. We also analyze the geometry of the system's motion as well as establish some properties of the motion of its center of mass. The findings of the paper extend corresponding results [9] in the dynamics of a rigid body to a case of the multibody chain as well as generalize some of the known results [8, 10] in the dynamics of many bodies.

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# Existence and Continuation Theorems of Caputo Type Fractional Differential Equations

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Recently, fractional differential equations (FDEs) have become a hot topic for its wide applications in many areas of sciences and engineering. However, the development of existence and uniqueness of solution of FDEs are very slow. Some contributions about existence of solution of FDEs on the finite interval $[0, T]$ can be found in [1, 2, 3, 4]. But few researchers [5, 6, 7, 8] found interesting results about the global existence-uniqueness of solution FDEs on half axis $[0, +\infty)$. In this talk, we consider the fractional order initial value problems (IVPs) in the following form

$$\begin{cases} {}_CD^{\alpha}_{0,t}\ x(t) = f(t, x), \quad 0 < \alpha < 1,\ t \in (0, +\infty), \\ x(t)|_{t=0} = x_0, \quad x \in R. \end{cases} \tag{1}$$

For the system of equations

$$\begin{cases} {}_CD^{\alpha}_{0,t}\ x_1(t) = f_1(t, x_1, x_2, \cdots, x_n), \quad 0 < \alpha < 1,\ t \in (0, +\infty), \\ {}_CD^{\alpha}_{0,t}\ x_2(t) = f_2(t, x_1, x_2, \cdots, x_n), \quad x \in R^n, \\ \cdots \\ {}_CD^{\alpha}_{0,t}\ x_n(t) = f_n(t, x_1, x_2, \cdots, x_n), \\ x_i(t)|_{t=0} = x_0, \quad i = 1, 2, \cdots, n, \end{cases} \tag{2}$$

where ${}_CD^{\alpha}_{0,t}$ is the Caputo derivative, $f : R^+ \times R \to R$ in the IVP (1) and $f_i : R^+ \times R^n \to R^n$ in IVP (2) have weak singularities with respect to $t$ respectively. In this talk, firstly, we establish the local existence for IVP (1) and IVP (2). Then we extend the continuation theorems for ODEs to those of FDEs. Furthermore, we present global existence of solutions for IVP (1)

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# Hopf bifurcation and stability analysis in delayed neural networks

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In this paper, delayed bidirectional associative memory (BAM) neural networks and ring networks are considered. BAM networks are able to store multiple patterns, but most of neural networks have only one storage pattern or memory pattern. BAM neural networks have practical applications in storing paired patterns or memories and possess the ability of searching the desired patterns through both forward and backward directions. It should be noted that periodic solutions can be resulted from Hopf bifurcation in delayed differential equations. The study of Hopf bifurcation is very important for the design and application of BAM neural networks because a great number of periodic solutions indicate multiple memory patterns. The delayed BAM neural network is described by the following system:

$$\begin{cases} \dot{x}_i(t) = -\mu_i x_i(t) + \sum_{j=1}^{m} c_{ji} f_i(y_j(t-\tau_{ji})) + I_i & (i = 1,2,\ldots,n) \\ \dot{y}_j(t) = -\upsilon_j y_j(t) + \sum_{i=1}^{n} d_{ij} g_j(x_i(t-\sigma_{ij})) + J_j & (j = 1,2,\ldots,m) \end{cases} \tag{1}$$

where $c_{ji}$ and $d_{ij}$ are the connection weights through the neurons in two layers: the X-layer and the Y-layer. The stability of internal neuron processes on the X-layer and Y-layer are described by $\mu_i$ and $\upsilon_j$, respectively. On the X-layer, the neurons whose states are denoted by $x_i(t)$ receive the input $I_i$ and the inputs outputted by those neurons in the Y-layer via activation function $f_i$, while the similar process happens on the Y-layer. Also, $\tau_{ji}$ and $\sigma_{ij}$ correspond to the finite time delays of neural processing and delivery of signals. Some authors have studied the dynamical behaviors of simplified forms of Eq. (1) (see e.g. Refs. [1, 2]). In fact, the authors considered models with a determined number of neurons. However, without any assumptions on the number of neurons, the dynamics of a general class of BAM neural network, containing one neuron in the X-layer and other neurons in the Y-layer is discussed in this paper that has not been done before.

A ring network is a network topology in which each node connects to exactly two other nodes, forming a single continuous pathway for signals through each node a ring. Data travel from node to node, with each node along the way handling every packet. Ring networks have been found in a variety of neural structures. In the field of neural networks, rings are studied to gain insight into the mechanisms underlying the behavior of recurrent networks. It should be noted that various local periodic solutions can arise from the different equilibrium points of ring networks by applying Hopf bifurcation technique, therefore the study of Hopf bifurcation is very important. In Ref. [3], Wang and Han investigated the continuous-time three-neuron bidirectional ring network model. Four-neuron and five-neuron networks with multiple delays have been also studied. Here, in this paper, the methods are generalized to study Hopf bifurcation on ring networks with arbitrary number of neurons and delays (not for a special number). To the best of our knowledge, it has not been done up to now.

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# Nonstandard Finite Difference Scheme for Vector Disease Models

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Epidemic models are normally solved using standard numerical integrators like the Euler and Runge-Kutta methods and other finite difference schemes. These standard methods fail to preserve the dynamics of the nonlinear differential equations and this can lead to spurious solutions. This is because of numerical instabilities that arise for certain values of the model parameters. This paper applies a nonstandard finite difference method to solve a vector disease model that preserves the positivity as well as maintaining the qualitative stability of the nonlinear differential equations. In particular, the Mickens' rule is used to approximate the nonlinear terms in the system of differential equations in a non-local way thereby considering some other terms in an implicit way. The results show that the nonstandard finite difference scheme is ideal in solving epidemic models as it preserves and obeys the dynamics of the nonlinear differential equations.

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# The Effect of Water Vapour Feedback as a Greenhouse Gas on a Simple Slab Model of the Earth's Atmosphere

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Around 3 to 5 million years ago in the Pliocene, the globally averaged temperatures of the Earth were warmer than they are in today's age. The external factors that determine today's climate are essentially the same as they were during the Pliocene. One of the most recognized contributors to the Earth's climate are the greenhouse gases. The main greenhouse gases are notably, carbon dioxide and water vapour. Water vapour feedback will be analysed in a simple slab model to determine the effects of the feedback alongside well known ice-albedo feedback and warming due to carbon dioxide. This slab model is applied to the Arctic region to investigate polar amplification due to water vapour feedback. The model is also applied to the Equatorial and Antarctic regions. This model also addresses the Pliocene paradox, suggesting why a warmer climate under the same conditions might have existed.

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# Two Sides of Delayed Dispersal in Metapopulation with Allee-like Effect

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Many species exist as "metapopulations" [1], that are collections of local populations connected by dispersal. These species persist because the extinction of local populations is counterbalanced by recolonization events that follows a dispersal event [2]. Our goal is to contribute to a more complete theoretical understanding of metapopulations dynamics by focusing on the heretofore-neglected role of delayed natal dispersal. We construct a model of a system of ordinary differential equations which includes a social structure (or hierarchy) within each local population, and we study the effect of delayed dispersal under the influence of birth rate and relative mortality rate of subordinates to dominants. We show that in our metapopulation system, there always exists a trivial extinction equilibrium, which is locally asymptotically stable, and that there are two additional non-trivial equilibria if and only if the determinant is positive; one of the equilibria is locally asymptotically stable, and the other is unstable. The stability of the trivial equilibrium indicates a strong Allee-like effect, or positive density dependence. The existence of a stable non-trivial equilibrium gives a condition for the persistence of metapopulations, where the two sides of delayed dispersal are revealed (see Fig. 1). Our model may provide some insight to a possible soluation

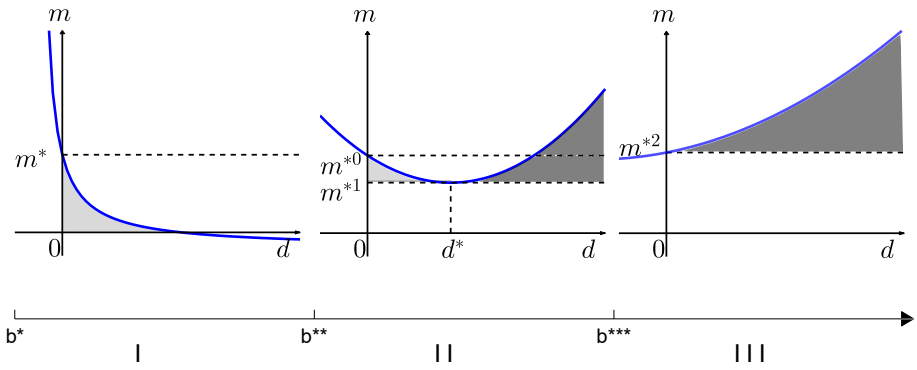


Figure 1: Two sides of delayed dispersal: delayed dispersal does help with the persistence of metapopulations in two regions with lighter shade on the left, but does not help in two regions with darker shade on the right, where higher dispersal rate helps. In other words, if the birth rate is low, with low mortality rate, delayed dispersal would be a better strategy for the metapopulation to persist; if the birth rate is in the level of moderate to high, movement corridors may benefit the metapopulation. The curves are sketched to show where sign changes for the determinant of the existence of non-trivial equilibria. Valid range of birth rate $b$ is separated to three intervals by critical values $b^*$, $b^{**}$, and $b^{***}$, and other values with a $*$ are also the critical values of relative mortality rate $m$ and dispersal rate $d$.

to an on-going debate among conservation biologists about the effectiveness of dispersal corridors on connecting fragmented local populations and to counter extinction, which involves proper distribution of finite economic resources of conservation.

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# CS-ENV Mathematical Modeling in Environmental Sciences and Models for Complex Media

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# A Comparative Study of Diffusion Term Appearing in Various Nonlinear Gas Transport Models in Tight Rocks

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Over the past few decades, various nonlinear gas transport models are used to describe the gas flow in tight porous rocks. Different modeling approaches are employed to develop these gas transport models. These approaches include the consideration of various flow regimes that occur in the tight porous rocks, such as viscous, slip, transition and free molecular flow, and the amount of adsorbed gas and free gas present in the reservoir. Different reservoir properties including gas density, gas viscosity, intrinsic permeability, tortuosity, porosity and many compressibility coefficients, are analyzed as pressure independent or pressure dependent. These modeling approaches lead to nonlinear gas transport models which differ in their diffusion terms. We investigate the effects of these diffusion terms on the distribution of pressure in the gas reservoirs. The results show that the better prediction of the pressure distribution in the reservoir is obtained by incorporating the full pressure dependent properties of the reservoir parameters.

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# Anticipating critical transitions in socio-ecological systems

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Abrupt and often irreversible transitions can be observed in a wide variety of systems including ecological communities, complex disease and social networks. Despite their seemingly unpredictable nature, generic early warning signals have been proposed [1], which once verified for a particular system, could provide the means for preventing unwanted transitions. However, these early warning signals rely on a phenomenon known as critical slowing down, which entails an increasing return time to equilibrium as a threshold is approached. The following hurdles motivate our research.

(i) Critical slowing down may occur only in very close proximity to the critical transition [2], meaning that any signals detected are most likely too late.

(ii) Complex systems possess multiple variables, some easier to measure than others. Not all may give early warning signals, despite being strongly influenced by the critical transition [3].

In response to (i) we develop necessary and sufficient conditions for pre-transition critical slowing down with a generic modelling framework that encompasses a wide range of simple ecological models. We show that these systems exhibit a critical slowing down as a critical transition is approached, provided the current stable equilibrium does not evolve at a rate exceeding a threshold value that is dependent on the basin of attraction. With regards to (ii) we show that the absence of early warning signals in certain variables can be explained using theory from multi-dimensional stochastic processes [4]. Harnessing this theory, one can infer which variables will exhibit the common traits of an upcoming transition. We apply this to some generic socio-ecological systems and demonstrate that sometimes signals in the ecological subsystem are silent.

Ecological systems are particularly fragile to human behaviour. When coupled to human dynamics, these systems can undergo a wide range of critical transitions, some with drastic, long-lasting consequences [5]. Prediction of these transitions before they arrive could allow time for control strategies that mitigate or completely avoid unwanted transitions. Our work sheds light on the mechanisms that suppress / exemplify early warning signals in these systems, and suggests that monitoring shifts in human behaviour is vital for the sustainability of ecological systems.

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# Characterization of Complexity in Anaerobic Digesters using Fractal Analysis

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Anaerobic digestion (AD) is a biological process that degrades organic materials and leads to the formation of biogas (a mixture of carbon dioxide and methane). AD is accomplished by a series of biochemical transformations in the absence of oxygen through four main steps, namely hydrolysis, acidogenesis, acetogenesis and methanogenesis [1]. In the hydrolysis step complex substrates are converted in simpler substrates. After that, in the acidogenesis step, available organic components are converted into organic acids, alcohols, hydrogen, and carbon dioxide by acidogens. In the acetogenesis step, the products of the acidogenesis are then converted into acetic acid, hydrogen, and carbon dioxide. Finally, methane is produced by methanogenic bacteria from acetic acid, hydrogen, and carbon dioxide as well as directly from other substrates of which formic acid and methanol are the most important.

Although this technology has been applied for several decades, there is still a lack of fundamental knowledge on the mechanisms of AD, what is mainly due to the very high complexity of the process. Indeed, as AD is a biological process, it is strongly influenced by several factors [1]. For instance, hydrolysis is the rate-limiting step for complex organic substrates, due to the formation of toxic by-products and volatile fatty acids (VFA). For easily biodegradable substrates methanogenesis is the rate-limiting step. Problems such as low methane yield and process instability are also often encountered in AD, preventing this technique from being widely applied. Finally, a wide variety of inhibitory substances are the primary cause of AD upset or failure since they are present in substantial concentrations in wastes.

Recent studies show that using fractal analysis of pH time series from AD reactor units it is possible to obtain correlations between the physical variables and fractal parameters [2,3]. This work focuses on the study of the correlation of fractal parameters (i.e., fractal exponent and fractal dimension) with the operational complexity of AD processes. This is done by using the rescaled Hurst fractal analysis, which is a method designed for the detection of correlations in complex time series [4]. Indeed, the fractal analysis has been an effective diagnostic tool in the study of biological complex fluctuations, efficient in handling noise and robust to detect correlations between variables [5]. We find a direct correlation between time-series complexity with the operational stability of AD processes.

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# Competition between injunctive social norms and conservation priorities gives rise to complex dynamics in a model of forest growth and opinion dynamics

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As human activities lead to declines in natural ecosystems, the decline in natural ecosystems can in turn stimulate human action to conserve endangered human ecosystems or attempts to restore badly damaged ecosystems [2]. Here, we develop a simple differential equation model in a coupled human environment system to evaluate the influence of injunctive social norms and gain general insights applying both qualitative as well as quantitative analysis. We consider the human perception of the conservation priority of a forest system depend upon how rare the ecosystem is.

Our opinion dynamics is based on [1]. We consider that a non-conservationist $1-x$ sample conservationist $x$ at a rate and switch to their strategy if perceived payoff gain of the other strategy is higher and vice versa. In addition we were interested to see the influence of injunctive social norms which impose a uniform pressure to remain in the same opinion state. We are also interested to quantify the effect of human forest harvesting versus slow rate of natural succession of forest. The equations are given by

$$\dot{x} = \kappa x(1-x)[c - F + \delta(2x-1)], \tag{1}$$

$$\dot{x} = RF(1-F) - h(1-x)F. \tag{2}$$

In this paper, we compare the results of the models with injunctive social norms and without social norms. The presence of injunctive social norms unexpectedly affects the stability and dynamics. In general, if human opinion is based only the costs of conservationism weighed against the rarity of the ecosystem, the two extremes of complete forest destruction and full forest cover are unusual outcomes. However, injunctive social norms make these outcomes more probable because when a norm of conservationism or non-conservationism is universally accepted, it tends to persist for long time [3]. At this point the conservation value of rare ecosystems is overshadowed by social psychology.

We have constructed a Dulac function in each case to rule out the possibility of the periodic orbit. The global stability of the interior state of mixed land in the presence of social norms is linked with complex constraints whereas it is unconditional in particular case.

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# Forest transitions, land use, and ecological thresholds

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The forest transition refers to a shift from net deforestation to net afforestation, which has occurred as a result of agricultural intensification and/or forest conservation in many countries [6]. Ensuring that forest cover does not continue to decline in countries that have not yet undergone a forest transition is key to protecting the ecological and economical value of forests, in addition to remaining within the "safe operating space for humanity" with respect to biodiversity, land use, and nutrient cycles [5]. However, human activities including agriculture, urban development, and lumber harvesting continue to encroach on forests [1], which may face additional strains from climate change. Models have been developed to predict future land use and define management strategies [3, 4]; however, these neglect established findings showing ecological thresholds in forest cover [7, 8]. We develop, analyze, and fit a nonhomogenous differential equation model of land use, incorporating ecological thresholds, to investigate the effects of these feedbacks, the risk of forest collapse, and management strategies.

This model displays a cusp bifurcation corresponding to forest collapse, which can be triggered by changes in several parameters. The forest cover at the bifurcation is consistently 20-30% even for widely varying parameters, suggesting an important management threshold in line with pre-existing guidelines [2]. Bifurcation diagrams and simulations highlight the importance of targeting land conversion rates as long-term targets, due to the greater sensitivity, and demonstrate that changes due to global warming threaten to compound pressure from agriculture. Ensemble simulations of time series near collapse indicate a subtle distinction between forest cover and forest resilience, indicating cases where one or both can be improved at no loss to agriculture. While agricultural land sparing and a reduction in forest clearing rate may intuitively seem to have similar impacts, these simulations allow us to identify scenarios where a particular choice is more effective in achieving a forest transition.

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# Impact of Spatial Structure and Human Dynamics on Environment Systems

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Coupled human-environment systems (HES), such as human-impacted landscapes, have complex dynamics that must be understood in order to facilitate effective conservation and land-use management. Progress has been made in modelling the dynamics of these systems, both in spatial and non-spatial settings. Spatial structure and the coupling of a human system to the environment system, have been shown to qualitatively alter model behaviours [1, 2, 3, 4]. However, as yet, there has not been a systematic analysis of how these model features interact to impact system dynamics and stability. We compare a non-spatial differential equation (DE) model of a human impacted landscape, to a spatially-explicit agent-based model (ABM) of the same system [3]. This is done in the presence and absence of human system dynamics in order to gain insight into how changes in these aspects of model structure impact system stability.

We begin with a DE model coupling transitions between forested and grassland states, to changes in the proportion of the human population which prefers the forested to the grassland state [3]. A spatially-explicit ABM analog of this DE model is formulated by converting rates of change to probabilities, and making transitions dependent on local proportions of land states and human preferences instead of the population-level proportions used in the DE model. The well-mixed system of the DE model is replaced by a landscape of discrete land parcels arranged on a 2-D lattice with periodic boundary conditions. The stability of these models is analysed in different regions of parameter space, both for parameters controlling transitions in the environment system, and the human system. We compare and contrast the results of this analysis for each model to examine how these aspects of model structure influence system dynamics.

This work contributes to a more complete understanding of how adding spatial structure and human dynamics to HES models impact stability outcomes. These insights will allow us to make better informed choices when constructing HES models, and enhance our ability to interpret the results of such models. Beyond the field of mathematics, an improved understanding of system dynamics will play a part in increasing confidence in HES model predictions, and facilitate their use as a tool for policy-makers developing environmental legislation.

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# Large eddy simulation of turbulent flow over a hill using a Canopy stress model

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Mathematical modelling of a turbulent flow over hilly terrains is an important topic in both mesoscale weather prediction and boundary layer meteorology. In comparison to the classical terrain following coordinate approach, Chow [1] demonstrates that the immersed boundary technique on a Cartesian grid simplifies the implementation of the boundary condition on the surface of the hill, and this approach also mitigates discretization errors which would occur due to the terrain following coordinate transformation [1]. In the present research, we have extended a canopy stress model to formulate the boundary condition on the surface of a hill, and considered the large eddy simulation method to predict the interaction between the near surface coherent structures and a smooth hill (see [2]). In addition to the canopy stress model, the turbulent stress has also been varied dynamically as the surface is approached, where the canopy stress model is derived based on the experimental observation that the drag coefficient becomes independent of the Reynolds number $(Re)$ when $Re$ is sufficiently large. The proposed model has been tested by simulating a neutrally stratified atmospheric boundary layer over a periodic array of smooth hills. As depicted in Figure 1, the agreement among the results of the present simulation, a dynamically similar experiment, and an equivalent numerical model suggests the potential benefits of the proposed method of simulating turbulent flow over hilly terrains.

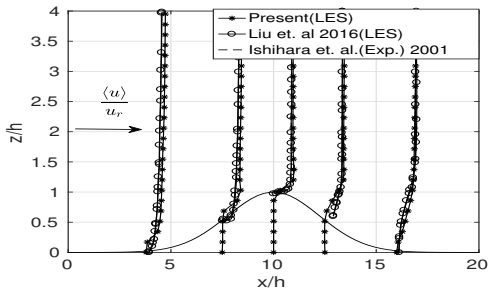


Figure 1: Comparison with the previous researches of the LES simulations of a different turbulent stress model [3] and an experimental results [4].

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# Modeling and Simulation of an Anaerobic Digester Treating Solid Organic Wastes

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Organic solid wastes (OSW) are commonly disposed of in landfills. However, due poor controlled conditions environmental problems can arise, including the methane emission, an essential contributor to global warming [1,2]. A promising alternative to treat OSW is to digest its organic matter employing the anaerobic digestion (AD). Indeed, AD is very suitable because of its limited environmental impacts and high potential for energy recovery [2,3].

Anaerobic single-phase systems, in which all main stages of AD (hydrolysis, acidogenesis/acetogenesis, and methanogenesis) take place simultaneously in a single reactor have been commonly used for the majority of waste [3,4]. However, since OSW undergoes rapid acidification resulting in the inhibition of methanogenic activity, two-phase anaerobic systems of different configurations and combinations of acidification and methanogenic reactors have been used by several authors for the treating of OSW [2,4]. These AD units differed mainly in the way microorganisms were retained in the bioreactor and the phase separation of main stages of AD.

Many papers have been published regarding the performance of single and two-phase AD units digesting OSW [1,4]. However, only a few papers have addressed the modeling including the particle size and biodegradability of the OSW. The ADM1 has been used as the reference of descriptive models capable of presenting good predictions on the performance of AD units [5,6]. However, due to its complexity, it is hard to calibrate completely, and also it is not appropriate for optimization and control design purposes.

In this work, we have developed a mathematical model of a single AD unit where the main stages of the AD are separated and sequentially performed. This configuration is favorable to avoid acidification problems. The mathematical model is described by a set of non-linear PDE and includes most important aspects of the AD, i.e. substrate biodegradability and particle disintegration, as well as main species involved at the hydrolysis, acidogenesis/acetogenesis, and methanogesis stages.

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# On Implementation of a Pseudo-potential Model in the Meshless Lattice Boltzmann Method

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Numerical simulation of multi-component and multiphase flows through porous media has a lot of scientific and engineering applications. For instance, flow simulation in groundwater and oil and gas extraction and recovery could be mentioned. Such simulations require efficient numerical techniques to solve the governing equations and to handle the complex computational domains [1].

The lattice Boltzmann method (LBM) has been used successfully for the simulation of different complex fluid flow problems in the past three decades. In particular, the LBM is considered to be an efficient solver for multi-component and multiphase flows. However, it suffers from some intrinsic restrictions. One of the major restrictions of this method is the difficulty in handling curved or irregular boundaries accurately. The situation gets worse and might need prohibitively large amount of computer memory in domains as complex as porous media or packed beds.

Recently, the authors have introduced a meshless scheme [2, 3] to eliminate the need for any mesh in the lattice Boltzmann method. As a result, geometrically complex flows (e.g. flows in porous media) could be solved using significantly lower computational resources [3]. However, the original meshless lattice Boltzmann method cannot handle multi-component and/or multiphase flows.

In this paper, the mathematical derivation and preliminary results of a new multiphase meshless lattice Boltzmann method are presented. First, the implementation of a pseudo-potential model [4] in the meshless lattice Boltzmann solver is discussed. Second, some numerical results for two benchmark multiphase flows are given. These benchmarks include the Laplace and the phase segregation test cases which are successfully simulated using the proposed model. The mathematical challenges of implementing the non-local collision term of the pseudo-potential model in the meshless method are also discussed. The paper presents the highlights of the mathematical and numerical issues involved in the derivation of the new model and presents early results of more complex flow simulations using the proposed meshless model.

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# Spreading of Near-shore Effluent Discharges on Eroded Sloping Sandy Beaches

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Coastal sewage treatment plants, power generation stations, and seawater desalination plants discharge their effluents through an outfall that stretches far into the ocean. The near-shore effluent discharge plumes are observed to be heading and spreading towards the shoreline, and may cause a build-up of concentration to higher levels in the coastal waters. Physically, the coastal area is a dynamic region where land and sea meet, and the sloping sandy beach is changing because of erosion and sediment transport in response to waves, winds, storms and sea level rise. Since erosion is causing the sand particles to move alongshore and/or drift out to sea, the summer (non-eroded) sloping sandy beach profile is reported to be changing to the winter profile due to eroded sediment is being deposited and accumulated offshore.

A simple far field modeling study is presented to evaluate the effect of erosion of a sloping sandy beach upon mixing and dispersion of the outfall effluent discharges, where the seabed depth profile is modelled as the power functions of distance from the beach. The two-dimensional advection-diffusion equation with a point source is analytically solved and illustrated graphically by plotting contours of solution to replicate the dispersion of effluent plumes discharged from a (single port) outfall (see Fig. 1). In terms of the practical applicability, it is well recognized that these kinds of mathematical models can be applied as a tool to perform quick preliminary worst-case assessments. If this easy-to-use assessment indicates no far field impacts at all, no further action is needed and the use of more sophisticated and time-consuming three-dimensional hydrodynamic and water quality modeling can be avoided.

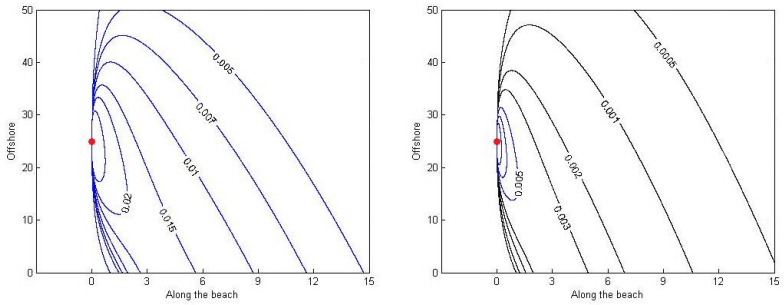


Figure 1: Effluent discharge plumes on an eroded (*left*) and a non-eroded (*right*) sloping sandy beach.

The maximum value of the shoreline concentration is formulated and used as an environmental impact measure that should not be exceeded anywhere along the beach to control public health risks in the areas where coastal waters is used for the recreational purposes. It is found that the significant increase in maximum concentration value (above the non-eroded sloping sandy beach) due to erosion cannot be reduced by extending the outfall pipeline alone.

Economically, it is cheaper to install a multiport diffuser (consisting of many closely spaced ports designed to discharge a series of effluent streams) at the end of the outfall pipeline rather than extending the outfall length. Reformulation of the model solutions using multiple point sources show that the increase in maximum concentration value can be eliminated by adding more ports. Thus, through a simplified mathematical model, it is demonstrated that the modern sea outfall systems with multiport diffusers do produce less potential environmental impact.

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# Temperature Effect on Sound Scattering by Fine Bubbles in Viscoelastic Liquid

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The presence of fine bubbles is a characteristic feature of polymeric solutions and melts because self-evacuation of free gas in such systems is complicated by usually high viscosity. Final properties of polymeric products are sensitive to small gas inclusions; therefore, diagnostics of microbubbles is an important part of different technological processes. One of the potentially efficient diagnostic methods is based on the acoustic technique, using registration of sound waves scattered by bubbles. Theoretical background of such technique for polymeric fluids with an emphasis on the liquid rheology impact on bubble dynamics was developed in a number of studies, summarized in [1]. Non-linear scattering of sound by gas bubbles with an account for liquid viscoelasticity was described in [2] in quadratic approximation; note also important contribution [3]. The existing results relate to isothermal conditions, so the question of the liquid temperature influence on sound scattering by bubbles is still open. The current analysis is focused on this question; it is supposed that in the studied temperature range the interface mass transfer has a minor effect.

It is assumed at the model formulation that dissipation features and nonlinearity at acoustic wave propagation in a quiescent polymeric liquid can be neglected. The spherical bubble in a sound field with the frequency $\omega_0$ is considered as a monopole type scatterer and the equation for its radius $R(t)$ is written in the form:

$$\rho(R\ddot{R} + 3/2\,\dot{R}^2) = \Delta p_g - p_a + \frac{2\sigma}{R_0}(1-\frac{R_0}{R}) + \tau_R\,, \qquad (1)$$

where $\tau_R$ is the liquid normal stresses input in the dynamic boundary condition at the bubble wall, calculated from the rheological equation for viscoelastic liquid with a discrete relaxation spectrum:

$$\tau_{ij} = 2\int_{-\infty}^{t} G(t-t_1)s_{ij}(t_1)dt_1 + 2\eta_s s_{ij}\,,\ G(t-t_1) = \int_0^{\infty} F(\theta)e^{-(t-t_1)/\theta}d\theta,\ \ F(\theta) = \sum_{k=1}^{n} G_0\delta(\theta-\theta_k)\,. \qquad (2)$$

The normalized scattering cross-section of the bubble at the basic frequency $\omega_0$ and nonlinear cross-section at the frequency of second harmonics $2\omega_0$ are calculated and studied numerically for macromolecular liquids with different polymer concentrations in a wide temperature range (which was chosen, however, far from the liquid boiling temperature). The temperature dependence of the rheological parameters is accounted for on the basis of Spriggs approximation for relaxation times distribution and the time-temperature superposition principle. The results indicate that the main effect of the temperature growth is localized in the vicinity of the bubbles resonance frequency and reveals itself in the scattering enhancement with temperature. Temperature dependence of the resonant frequency and the impact of polymer concentration are studied as well.

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# Turbulent Diffusion of Inertial Particle Pairs Such as in Pollen and Sandstorms

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Inertial particle pair diffusion has received less attention than fluid particle pair diffusion, even though it is more relevant to real world applications such as sandstorms, and pollen dispersion. Only the DNS of Bec et al [1] has been reported. A non-local theory of fluid particle pair diffusion has recently been proposed [2]. Here, we investigate inertia pair diffusion numerically [3,4], in the limit of Stokes' drag where the transport is given by,

$$\frac{dx}{dt} = v(t) \quad \text{and} \quad \frac{dv}{dt} = -\frac{1}{\tau}(v(t) - u(t)), \tag{1}$$

$\boldsymbol{x}(t)$ is the particle position at time $t$, $\boldsymbol{v}(t)$ is the particle velocity, $\boldsymbol{u}(\boldsymbol{x},t)$ is the Eulerian velocity field generated by the Kinematic Simulation [3], $\tau$ is the particle response time. The Stokes number is, $St = \tau/t_h$, where $t_h$ is the Kolmogorov time scale, $\sigma_l(t) = \langle l(t)^2 \rangle^{1/2}$, where $l(t) = |\boldsymbol{x}_1(t) - \boldsymbol{x}_2(t)|$ is the distance between particles in a pair in an ensemble of particle pairs released at time $t=0$ such that $l(t=0) = l_0 < \eta$. $\eta$ is the Kolmogorov scale of the turbulence. For short times, the very small energy in the small scales of turbulence does not affect the particle relative motion, and we expect ballistic motion, $K_l \sim \sigma_l^{\,1}$, for $t << T^*$, where $T^*$ is some time scale. At large pair separations the turbulent energy will be dominant, and the diffusion will approach *fluid* pair diffusion, $K_l \rightarrow K \sim \sigma_l^{\,1.53}$, for $T^* << t << T_L$, [3] where $T_L$ is a timescale when their motions are independent. We expect an intermediate transition regime determined by when the local Stokes number, $St(l^*) = \tau/T^* = 1$. This leads to, $\sigma_l^{\,*}/\eta \sim St^{2/3}$ [1]. KS was used in a frame of reference moving with the (virtual) large scale sweeping velocities with spectrum, $E(k) \sim k^{-5/3}$, for $1 \le k \le 10^4$, and $E(k) = 0$, for $k < 1$. Fig. 1 shows the inertial pair diffusivity $K_l/\eta v_\eta$ against the pair separation $\sigma_l/\eta$ for a wide range of Stokes number, $0 \le St \le 50$. The results display short time ballistic regimes, and long-time non-local scaling, $K_p \rightarrow K \sim \sigma_l^{\,1.53}$, and an intermediate transition regime, as predicted by the theory. Fig. 2 shows $\sigma_l^{\,*}/\eta$ against $St$, displaying an approximate 2/3 scaling. We will report upon the completed work up to $1 \le k \le 10^6$ at the time of the conference

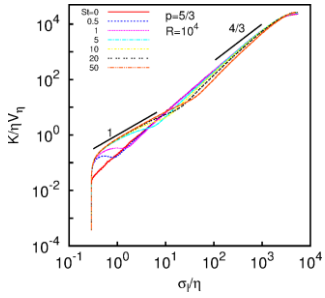


**Figure 1:** Pair diffusivity against the pair separation.

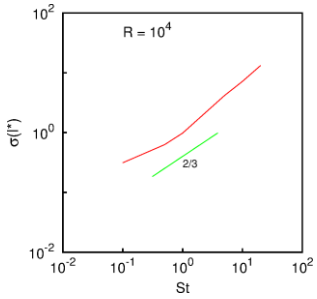


**Figure 2:** Transition point against the Stoke's number

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# CS-FINANCE Financial Mathematics and Computation

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# Algorithms for Flow Trades at NASDAQ around its Close

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In this talk, we analyze how an investor optimally executes a large stock order at NASDAQ when the closing price is the benchmark. For many investors, particularly managers of mutual funds, the closing price of a stock is an important benchmark. In mutual funds, flow trades correspond to inflows or outflows of cash when clients decide to buy or sell shares of the fund. Regardless at which specific time the transactions are taking place on any trading day, the mutual fund managers will receive from or pay to the client the closing price. Hence, such traders use the closing price as their benchmark: they aim to achieve a price that is as close as possible to the closing price and, if possible, more favourable than the closing price. The closing price for stocks traded at NASDAQ is determined through an auction, like at many other stock exchanges. Each day and for each stock traded at NASDAQ, the intertemporal order imbalance of the auction is announced beginning ten minutes before the close.

We introduce a mathematical framework that takes the order imbalance announcements into account. Similarly to the classical setting in Almgren and Chriss [1], the investor's objective is to minimize a combination of expected slippage and standard deviation of slippage, but here with the closing price (instead of the arrival price in [1]) as the benchmark. The investor can place orders in the closing auction before the imbalance announcement as well as participate in the continuous trading before and after the imbalance announcement. The investor is guaranteed to receive the closing price if the total volume of the order is placed in the closing auction so that the slippage is zero.

We show, however, that the investor performs better overall by taking some risk and achieving a negative slippage on average when participating in the continuous trading as well. Under suitable assumptions, we find explicit formulas for the optimal trading strategy that have the following properties:

1. *The investor participates in the continuous trading before the imbalance announcement, in addition to submitting orders to the auction.*
   The investor's orders submitted to the auction have a market impact at the moment when the imbalance announcement is revealed. The investor trades before the imbalance announcement to benefit from prices which do not reflect the later market impact of the investor's own auction orders.
2. *It is not beneficial for the investor to trade after the imbalance announcement.*
   After the imbalance is announced, the impact of the investor's own participation in the closing auction is reflected in the prices. By participating in the continuous trading afterwards, the prices will not be favourable compared to the closing auction price, but reflect risk by contributing to standard deviation in slippage.

These mathematical findings are in line with observations discussed in Bacidore et al. [2]. Using real historical data, we simulate the performance of the proposed algorithm and find a small, but persistent out-of-sample improvement and a reduction in average trading costs.

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# High-order scheme for option pricing with stochastic volatility and jumps in returns

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Option pricing remains an interesting area of study for mathematicians driven by the demand for financial derivatives among traders and investors alike. We introduce a IMEX high-order compact finite difference scheme to compute options priced under the Bates Model [1]. The Bates model is a stochastic volatility model which allows for jumps in returns, posed by coupled stochastic differential equations we are able to apply standard derivative pricing arguments to obtain the PIDE

$$\frac{\partial V}{\partial t}+\frac{1}{2}S^2\sigma\frac{\partial^2 V}{\partial S^2}+\rho v\sigma S\frac{\partial^2 V}{\partial S\partial\sigma}+\frac{1}{2}v^2\sigma\frac{\partial^2 V}{\partial\sigma^2}+(r-\lambda\xi_B)S\frac{\partial V}{\partial S}+\kappa(\theta-\sigma)\frac{\partial V}{\partial\sigma}-(r+\lambda)V+\lambda\int_0^{+\infty}V(S\tilde{y},v,t)p(\tilde{y})\,\mathrm{d}\tilde{y}.$$

Following the method employed by Salmi and Toivanen [3], we accomplish the implicit-explicit discretisation in time by means of the IMEX-CNAB method. This method is an adaptation of the Crank-Nicholson method, whereby an explicit treatment is added for the integral operator, after a two-step start-up the IMEX-CNAB steps are defined as

$$(\Delta\tau L_D)\,u^{n+1}=\left(\Delta\tau L_D+\frac{3\Delta\tau}{2}L_I\right)u^n-\left(\frac{\Delta\tau}{2}L_I\right)u^{n-1}.$$

To achieve high-order convergence we utilise the finite difference scheme used by Düring, Fourniè [2] to implicitly compute the differential operator, $L_D$, while we evaluate the integral operator $L_I$ explicitly using Simpson's rule. The scheme is coded using C++ with use of the GSL libraries.

In addition to a discussion of the methodology used we will present the results of numerical experiments, which examine the convergence, see Fig. 1, and the stability of the scheme. We will also discuss how this new high-order scheme can be beneficial to financial practioners as well as being incorporated into their existing models.

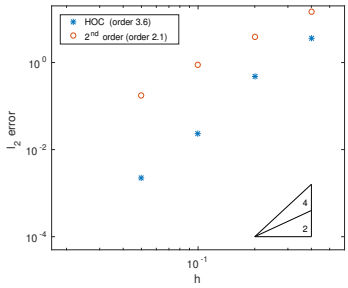


Figure 1: Comparative $l_2$ norm of high-order and 2nd-order schemes.

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# Implying jump-diffusion model pricing parameters with an optimal control approach

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A widely publicized criticism of the Black-Scholes option pricing model is that it fails to model the volatility 'smile/skew'. This phenomenon describes the apparent dependence of the volatility parameter on the option's strike price and time to maturity. Option pricing models have grown in complexity over the years, at least partly to take account of this schism. Dupire [1] presented the forward Black-Scholes equation, modelling the 'local volatility' as a deterministic function of an options strike price and maturity. Later, Andersen and Andreasen [2] extended this approach by deriving a forward partial integro-differential equation based on the jump-diffusion pricing model, originally introduced by Merton [3], which incorporates a local volatility function along with a random jump term. The jump term intends to take account of the discontinuous behaviour of the underlying asset.

We aim to approximate the local volatility function and the jump term's Poisson parameter simultaneously by reformulating the problem as a distributed optimal control problem, treating the forward PIDE as our state equation. By approaching the problem with the analysis of optimal control theory, we may investigate the necessary regularity conditions for our parameters of interest. We therefore prove the existence of unique optimal solutions under certain analytical conditions. Furthermore, we establish the first-order necessary conditions for optimality. Using Lagrangian multipliers, we incorporate a cost function in order to regularize our parameters and compare our PIDE solution with market prices, and derive an adjoint equation along with inequality constraints to accompany the PIDE that governs the option price in order to fulfil the necessary conditions for optimal solutions. Such a Lagrangian-based optimal control approach has been applied in [4] to the forward Black-Scholes PDE and is successful at solely implying a volatility surface from market data.

Our numerical method uses a gradient descent technique to update the volatility surface and Poisson parameter. At each iteration we must solve the PIDE along with the adjoint equation using standard finite element methods and modify the parameters suitably. This method is applied until the necessary first-order conditions of optimality are met. Finally, results will be presented in the context of a validated forward PIDE model. The status of this work at the time of writing is that the numerical results are in the process of being acquired.

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# Methodology for Estimating Loss Given Default (LGD) and Probability of Default (PD) Correlations under Economic Downturn

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The provision in Paragraph 468 [1] for calculating Loss Given Default (LGD) requires that parameters used in Pillar I of Basel II capital estimations must be reflective of economic downturn conditions so that relevant risks are accounted for. This provision is based on the fact that the probability of default (PD) and LGD correlations are not captured in the proposed formula for estimating economic capital. To help quantify economic downturn LGD, the Basel Committee proposed establishing a functional relationship between long-run and downturn LGD.

Miu and Ozdemir [2] proposed a stylized model to map out this relationship and then proposed a method for estimating the parameters in the model. This study has shown that the proposed method is defective, which implies that the empirical findings based on this method will be defective as well. The flaw stems from estimation of model parameters from incorrect distribution. Our analysis indicates that the model-implied economic capital is extremely sensitive to their estimation error. In particular, the methodology leads to gross overestimation of economic capital (see Table 1). As such, any improvement to their estimation methodology would be a significant contribution. The objective of this project is to propose a novel method that may improve upon the proposed estimation methodology by Miu and Ozdemir [2].

| Percentage difference of Economic Capital | Correlation between *LGD* and Default Rate | | | | |
|---|---|---|---|---|---|
| | 0.0 | 0.2 | 0.4 | 0.6 | 0.8 |
| 99% | -2.63% | 16.33% | 25.55% | 21.98% | 12.05% |

Table 1: Percentage difference in economic capital based on incorrect and correct distributions at 99% confidence interval

The model proposed by Miu and Ozdemir [2] to establish a relationship between long-run and downturn LGD is divided into two categories – systematic risk and idiosyncratic risk models. These models have parameters that determine the degree of impact of both the systematic and idiosyncratic risk on portfolio losses. And are linked to PD and LGD correlations. As pointed out above, the estimation methodology proposed by Miu and Ozdemir is defective. This study investigates approaches to correct the defect in the estimation methodology by Miu and Ozdemir [2].

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# On Characterization of Option Price Boundaries via Comparison of Stochastic Processes and Market Completions

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As the focus of modern mathematical finance tends to shift away from the renowned Black-Scholes model to more complicated models, the problem of option price calculations becomes more and more apparent. It is commonly agreed that the classical log-normal process and its modifications do not allow for explicit calculations and they are not accurate enough for the real-world applications. That is why the problem of finding and/or approximation of the acceptable range of option prices becomes very important from both theoretical and practical points of view.

In the talk, we present two methods to solve such a problem.

First, we present the option pricing method which gives approximate formulas that are fast, easy to implement and yet very accurate. The approach is based on a path-wise comparison property of strong solutions of stochastic differential equations. We show how this method works for a class of financial markets with stochastic volatilities (CEV models).

Second, we present another approach consisting in a description of option price boundaries by means of market completions. In the framework of an incomplete multivariate diffusion market model we develop a dual theory of option pricing.

We provide numerical examples to illustrate both methods and to demonstrate their precision and advantage with existing methods.

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# One-dimensional Partial differential equations for Asian option prices

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In this talk, we consider fixed and floating strike European style Asian call and put options. For suchoptions, there is no convenient closed-form formula for the prices. Previously, Rogers and Shi, Vecer, and Dubois and Lelièvre have derived partial differential equations with one state variable, with the stock price as numeraire, for the option prices. In this talk, we derive a whole family of partial differential equations, each with one state variable with the stock price as numeraire, from which Asian options can be priced. Any one of these partial differential equations can be transformed into any other. This family includes four partial differential equations which have a particularly simple form including the three found by Rogers and Shi, Vecer, and Dubois and Lelièvre. Recently, Vecer derive a new PDE using the average asset as numeraire. We perform numerical comparisons of the five partial differential equations by Crank-Nicolson method and conclude, as expected, that Vecer's equations and that of Dubois and Lelièvre do better when the volatility is low but that with higher volatilities the performance of all five equations is similar. Vecer's equations are unique in possessing a certain martingale property and they perform numerically well or better than the others.

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# Stochastic Modeling of Asynchronous Assets with Jump-Diffusion Processes

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I this talk, we present new jump-diffusion models for dealing with financial securities that have missing or asynchronous data in time series of prices. This project is a continuation of [1] where the model based on a multivariate geometric Brownian motion (GBM) was constructed. The proposed models allow us to analyze a portfolio that combines a high-activity asset such as a market index (or an exchange-traded fund tracking a market index) and several low-activity assets. The models are constructed in such a way that low-activity assets correlate with each other only through the high-activity asset price process. For the calibration of models, we estimate parameters for a high-activity asset first and then estimate parameters for each low-activity asset conditional on the parameters for the high-activity asset.

Two cases are considered. First, jumps can only happen in the high activity asset process. The second case is where low-activity assets have jump-diffusion components that are independent of that for the high-activity asset. We consider both the normal and double-exponential distributions for jump sizes. We use the maximum log-likelihood method to estimate model parameters for different time-series datasets. The new models are compared with the one based on a multivariate Geometric Brownian motion. We also evaluate and compare the value at risk (VaR) and expected shortfall for all models using the Monte Carlo method.

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# Long-Term Optimal Portfolio Selection Problem

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In this project, we aimed to develop a complete methodology for finding the best investment portfolio, which is meeting risk preferences of an investor. To consider different aspects of their risk preferences, we used a combination of several risk and performance metrics as a ranking function. We also applied three different methods to evaluate the long-term value of those metrics for each fund. They are the static value method, the occupation-time method, and the occupation-area method. After applying the ranking system to select most suitable funds from a large pool, we use different models to find an optimal portfolio. Past 5-10 years data have been extracted using a Bloomberg terminal. We found that the asymmetric multivariate t-distribution can dominate the multivariate normal distribution and the symmetric t-distribution in capturing the market behavior. This has been demonstrated by calculating the likelihood function for each model. We also realize that using a linear combination of several risk or performance metrics can help us to select the most suitable portfolios lying on the efficient frontier that are meeting unique risk preferences of an investor.

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# CS-MECHE Computational Mechanics and Engineering

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# A computational Model for Adjusting Surface Tension Coefficient in Pseudo-potential Lattice Boltzmann Method

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The lattice Boltzmann method (LBM) has attracted a lot of attentions in recent years due to its various capabilities and merits. In particular, it has gained a popularity in simulating complex flows such as multi-component and multiphase flows as well as flows through porous media in a wide range of scales from macro to micro. Despite the rapid adoption of LBM for simulating complex flows, it still has some drawbacks and deficiencies, specially when dealing with practical applications. One of the widely used models for multiphase flow simulations is the pseudo-potential LBM introduced by Shan and Chen [1]. They introduced their model based on an interaction potential among particles which resulted in an automatic phase separation. However, the original model was limited to flows with small density ratios and produced large spurious currents.

To alleviate the limitations in the original pseudo-potential model, Yuan and Schaefer[2] brought a real equation of state (EOS) into the pseudo-potential function which improved the model performance noticeably. Later on, Kupershtokh et al.[3] proposed the exact difference method (EDM) and with the use of EDM and a real EOS they were able to improve the applicability of the pseudo-potential model. Recently, Hu et al. [4] and Xu et al. [5] have added extra parameters and force terms to enable their models to simulate multiphase flows with higher density ratios. However, all these improved models are still limited in adjusting the surface tension parameter in a rather narrow range and the surface tension could not be explicitly specified at different temperatures.

In this paper, the EDM in pseudo-potential model is modified to improve its applicability for more realistic flow simulations. The proposed modification is implemented by introducing a surface tension parameter, $k^{'}$, into the pseudo-potential function using a nondimensional real EOS. The proposed model is successfully applied for the simulation of a flat interface and the Laplace test. It is shown that the introduction of this new parameter has no adverse effects on the accuracy of the calculated densities of the two phases. By adjusting this parameter the surface tension is tuned in a wider range up to an order of magnitude larger. However, by increasing the surface tension the spurious velocities could increase. An equation is also introduced to explicitly determine an initial value for the surface tension through the pseudo-potential function which could be utilized at different temperatures.

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# A full waves structure Riemann Solver and Second-order Cell-Centered Lagrangian Method for Two-dimensional Elastic-Plastic flows

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For 2D elastic-plastic flows with the hypo-elastic constitutive model and von Mises yielding condition, the non-conservative character of the hypo-elastic constitutive model and the von Mises yielding condition make the construction of the solution to the Riemann problem a challenging task.

In this paper, treating the usual conservation laws of the volume, the momentum and the total energy and the hypo-elastic constitutive model as equal part of the hyperpolic system, we first analyze the waves structure of the Riemann problem and develop accordingly a four-rarefaction waves approximate Riemann solver with elastic waves (FRRSE). In the construction of FRRSE one needs to use an iterative method. A direct iteration procedure for four variables is complex and computationally expensive. In order to simplify the solution procedure we develop an iteration based on two nested iterations upon two variables, and our iteration method is simple in implementation and efficient. Based on FRRSE as a building block, we propose a 2nd-order cell-centered Lagrangian numerical scheme.

Numerical results with smooth solutions show that the scheme is second-order accurate. Moreover, a number of numerical experiments with shock and rarefaction waves demonstrate the scheme is essentially non-oscillatory and appears to be convergent. For shock waves the present scheme has comparable accuracy to that of the scheme developed by Maire et al Refs. [1], while it is more accurate in resolving rarefaction waves.

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# A High Accurate Algorithm for Diffusion Equations on Distorted Meshes

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In this paper, a new type of finite volume scheme for diffusion equations on distorted meshes is firstly established. When vertex quantities are presented as the linear combination of the surrounding cell-centered unknowns, the scheme is expressed as nine-point form on general quadrilateral mesh and degenerates to five-point form on regular quadrilateral mesh. Then, a new treatment for the vertex unknowns is developed with “twin-fitting" method, which provides global high accuracy of the method either at discontinuous points of the diffusion coefficient or not. At last, numerical experiments draw that the treatments for the vertex unknowns play a key role in determining the accuracy of the scheme, and show that the finite volume scheme with the new treatment has almost second order accuracy on distorted quadrilateral meshes and is priori to the schemes with other treatments.

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# Asymptotic Expansions for High–Contrast Linear Elasticity Problems

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There is a growing interest in the computation of solutions of problems governed by partial differential equations with high-contrast coefficients. Solutions to these model problems are multiscale in nature. The solutions to these problems are often approximated using the Finite Element Method (FEM), Multiscale Finite Element Method (MsFEM) or alternative forms of these, (cf., [2, 3] and references therein).

Herein, we study linear elasticity problems in heterogeneous media. Our goal is to devise approximate solutions that account for the high contrast in the coefficients. We focus on the dependence of the contrast in the coefficients where the contrast is referred to as the ratio of the jumps in the physical properties. We follow the analysis presented in [1] that consists of deriving an asymptotic expansion for the solution of the elliptic differential equation in heterogeneous media. Thus, we derive asymptotic expansions to solve linear elasticity problems with high contrast.

The linear elasticity equations model the equilibrium and the local strain of deformable bodies. The constitutive laws relating stresses and strains depend on the material and the process modeled. For composite materials, physical properties such as Young's modulus can vary several orders of magnitude and we seek to understand the effects of these variations on the solution. In this setting, the asymptotic expansions that express the solution are useful tools to understand the effects of the high contrast and the interactions between different materials, see [4]. We study the convergence of the expansion in the $H^1$ norm.

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# Dependence of turbulent Rayleigh–Taylor mixing on the complex initial perturbation

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As we known, in turbulent Rayleigh – Taylor flow (i) the mixing width of bubble h grows as $h(t)=\alpha Agt^2$, and (ii) the wavelength of dominant bubbles $\lambda$ grows self-similarly with h as $\lambda(t)=\beta h(t)$. Over the past two decades, a lot of experimental and numerical studies imply that both $\alpha$ and $\beta$ are not a universal constant, especially for mixing induced by complex initial perturbation involving long wavelength. For such problem, some researchers suggested that the mixing evolves dominantly through mode-competition mechanism. Up to now, however, no satisfactory formula for either $\alpha$ or $\beta$ has been obtained to reproduced the observed variation with the non-dimensional density ratio A and perturbation amplitude $h_0^*$. In this talk, we will report an analytical model to achieve this goal. The theory is derived by successively solving the evolution induced by single-mode, wave-packets and multi-mode perturbation. Our new theory predict that (i) $\beta(A)=(1+A)/4$ depends only on A, and (ii) $\alpha(h_0^*)=[2\varnothing/\ln(2h_0^*)]^2$ depends only on $h_0^*$, where $\varnothing$ is an equivalent coefficient to take account of the artificial numerical viscosity in MILES simulation and is unity in experiments. Our predictions agree very well with the series of simulations and experiments (i.e. Rocket Rig and LEM experiments) conducted in the broad range of $0\leqslant A\leqslant 1$ and $10^{-7}\leqslant h_0^*\leqslant 10^{-2}$. To the best of our knowledge, this is the first time that a theory successfully reproduce the dependence of $\alpha$ or $\beta$ on all A and broad $h_0^*$.

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# Genetic Algorithm Optimization for deriving Compact Thermal Models

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The miniaturization of electronic systems led to a dramatic increase of the amount of heat generated per unit volume. Despite continued advances in Computational Fluid Dynamics simulations, accurately predict the sensitive temperature of a semi-conductor at system level remains a key challenge. A way to address, this issue is the substitution of complex representation of electronic components, which need high computing resources by set of Compact Thermal Models. The concept of compact thermal model was defined, by the European consortium DELPHI in order to minimize the computation times, from days to minutes. Delphi compact thermal model resumes an electronic component as a simple cuboid form and a network of Boundary Condition Independent thermal resistors that links a single temperature-sensitive node to all major isothermal surfaces of heat extraction. The network building is based on a set of 38 "universal" heat transfer coefficients, defined by JEDEC, that are applied on these external surfaces. However, the DELPHI method requires a network solver, which enables to efficiently minimize the temperatures and heat fluxes errors of the derived surrogate model.

The presented work discusses the achieved performances of a set of Genetic Algorithms to generate the relevant parts of the surrogate model such as the subdivision of its frontiers[] that interact with its surroundings or the definition of resistances and capacitances values[] of the internal thermal network, as resumed Figure 1.

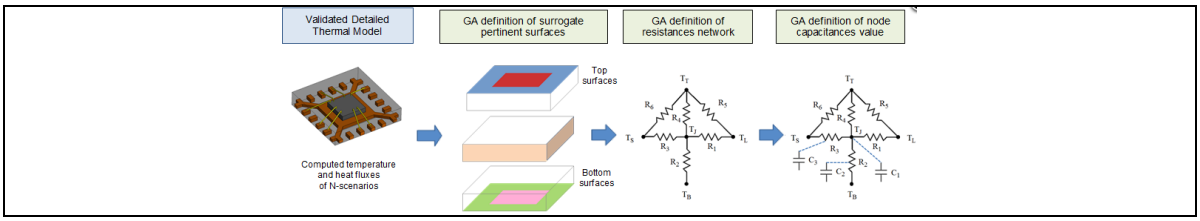


Figure 1: Process flow based on inspired-DELPHI compact thermal model creation.

Various optimizations on the significant GA parameters (cost function, elitism, population, crossover and mutation, global minimum research…) are highlighted in order to give an overview of the process robustness.

The resulting GA optimization routine provides a solution to obtain from numerical simulations a very simple surrogate model using usually less than 10 nodes. The derived low-node network allows us predicting the sensitive temperature and the leaving heat fluxes within a discrepancy lower than 10%, as reported in the following references.

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# Hardness Prediction of Particle-reinforced Metal Matrix Composite Materials

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Metal matrix composite materials (MMCs) are frequently used in different engineering applications, for example, cutting tools, automobile, aerospace, mining equipment, armors and functional materials [1,2]. By proper selection of production parameters, it allows the production of a family of MMC with specific hardness, fracture toughness and corrosion resistance to suit a wide range of operating conditions in industry [3,4]. Development of modeling methodology to simulate mechanical performance of MMCs and guide the selection of reinforce particle and host metal matrix is important for further advancing MMC technologies.

In this study, a conceptual model is proposed to calculate the hardness of particle-reinforced MMCs with its microstructure and production parameters considered. In the model, two scales of modeling are involved, namely micro-scale and continuum scale modeling. At micro-scale, a concept called representative equivalent volume (REV) is adopted to investigate the effect of heterogeneous microstructure on the equivalent mechanical properties of MMCs. At the continuum-scale, indentation process used in laboratory hardness testing is simulated by finite element method (FEM) based on the stress-strain curves obtained from the micro-scale modeling.

The simulated hardness is compared with the results from measurement and a good agreement is observed demonstrating the validity of the proposed model. In addition, the effect of different interface bonding scenarios is also investigated and discussed. Further parametric studies on production parameters and even material properties are suggested in the end to improve the MMC mechanical performance in the future.

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# MHD Flow in a Rectangular Duct

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The magnetohydrodynamic (MHD) flow of an incompressible, viscous and electrically conducting fluid is considered in a rectangular duct with different types of boundary conditions under the influence of a uniform external inclined magnetic field. The flow is fully developed and driven by a constant pressure gradient in the axial direction. The MHD flow in rectangular ducts has been intensively studied for various wall conductivities with no-slip conditions. However, there have been very few works on the solution of MHD flow with the slip condition although a slip boundary condition must be employed in some applications, e.g. microfluid and nanofluid devices, in which the slip behavior is typical when the surface to volume ratio is large. In these works with slip, a special case of MHD flow in a rectangular duct with either only perfectly conducting or non-conducting walls under a uniform transverse magnetic field is analytically analyzed. Therefore, the present study focuses on the numerical solution of the MHD duct flow with the most general boundary conditions involving both the variable wall conductivity and the mixed type slip boundary condition which is constructed as a linear combination of the slip velocity and the tangential stress. Moreover, the external magnetic field is inclined making a positive angle with the vertical axis. These are the main contributions of the present study. The nonlinear governing partial differential equations coupled in velocity and induced magnetic field are discretized by the boundary element method (BEM) which uses a fundamental solution that enables one to treat these equations in their original coupled form. The resulting system of equations involving the unknown values of velocity and induced magnetic field only on the boundary of the duct is small in size and is solved at one stroke with no iteration. Thus, the BEM results are obtained with less computational effort when compared to the domain decomposition techniques, which is one of the basic advantage of the BEM. The validity of the BEM code is also ascertained by comparing the present results with previously published analytical ones given for the MHD duct flow with non-conducting walls and slip condition in the presence of a horizontally applied uniform magnetic field. The numerical simulations are carried out for several values of slip length, Hartmann number, and also for the inclination angles of the external magnetic field. It is well-observed from the equivelocity and induced current lines that the flow is controlled by either MHD or slip effects according to the ratio of the slip length to the thickness of the Hartmann layer. That is, when this ratio is very small the flow shows no significant difference compared to the case of classic MHD flows without the slip whereas in the strong slip condition, when the ratio is large, the flow is controlled by the slip effects. On the other hand, the effects of both MHD and slip are significant when the ratio is of the order of unity.

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# On the Use of Lattice Boltzmann Method for Simulating Peristaltic Transport of a Single Solid Ellipsoidal Particle Suspended in a Newtonian Fluid

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Peristaltic transport refers to the flow of a fluid caused by periodic deformation of the flexible walls of a channel. Pumps devised based on this novel idea are widely used in industry for the transport of corrosive or sterile fluids. They are also well suited for the transport of high-solid slurries. The case of a fluid containing solid particles is also of prime interest in biomechanics where such a type of flow is normally encountered in the ureter of our urinary system for the transport of kidney stones. Although modelling peristaltic transport of viscous fluids has been the subject of much study in the past, it is only very recently that are we witnessing research in this area involving large solid particle(s). Of particular importance is the recent work by Connington et al. [1] who addressed the transport of a single circular solid particle in a viscous fluid. That work served to show the importance of the size of the particle and its initial positioning on its eventual fate. It also showed that the center state is not necessarily the most stable configuration for the particle. In spite of its importance, it should be conceded that not all particles are necessarily circular. The question then arises as to what would be the results if the particle is not circular. In this research, we consider peristaltic flow of a Newtonian fluid carrying a single solid particle of ellipsoidal shape. The particle, which is neutrally buoyant, is initially positioned on the centerline of a planar channel. Figure 1 schematically depicts the flow domain under consideration. The flow generated this way is assumed to be laminar and two-dimensional. To achieve this goal, the flow is simulated using the Lattice Boltzmann Method (LBM) coupled with the Smoothed Profile Method (SPM). Using this method, both the fluid dynamics and solid dynamics are efficiently computed on a fixed Eulerian grid. The Momentum Exchange scheme is also used for the interaction between the walls and the fluid. The role played by the aspect ratio of the particle is what interests us most in this challenging fluid mechanics problem. Based on the results obtained in this work, circular particles are better suited for peristaltic transport as compared with the ellipsoidal particles.

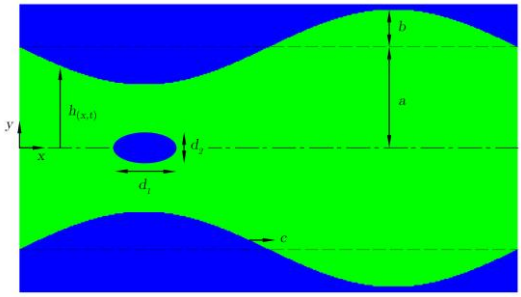


Figure 1: Schematic showing the flow geometry.

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# Optimization of flanged DAWTs using a CFD Actuator Disc Method

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For improving the efficiency of horizontal axis wind turbines, shrouded or ducted wind turbines have become state of the art research topics. Getting energy from a wind turbine more than the Betz limit is a great motivation for researchers. Recent Computational Fluid Dynamics (CFD) simulations or experimental tech-niques show the effects of dominant factors such as the length of the duct, the angle of the diffuser, and the height of the flange.

In the current study, a ducted wind turbine is simulated numerically combined with an Actuator Disc (AD) method. The first step is to find the maximum velocity in the duct by improving the angles of the flange to finalize the geometry of the duct. Then, the powers of the bare wind turbine and the Diffuser Augmented Wind Turbine (DAWT) are compared numerically while an AD method is used for modeling the rotor of the hori-zontal axis wind tubine. For the numerical simulation, the k-omega turbulent model is applied. For the 2D axisymmetric geometry, more than 0.5 million cells are used.

The results will show that the axial velocity can be enhanced more than 60 percent. The CFD analysis proves that the angle of the flange dominates the efficiency of the DAWTs and plays a key role in the enhancement of the power extraction of the horizontal axis wind turbines.

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# Performance, Thermal Stability and Optimum Design Analyses of Rectangular Fin with Temperature-dependent Thermal Properties and Internal Heat Generation

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In this paper, we numerically analyse the thermal performance, thermal sstability and optimum design of longitudinal fin with temperature-dependent thermal properties and internal heat generation under multi-boiling heat transfer using the Haar Wavelet Collocation method. The effect of various significant and controlling parameters on the thermal performance of the fin are investigated, established and discussed. In addition, the thermal stability criteria and optimum design parameter are established. The computational results obtained from the study shows that the effects of the thermogeometric parameter, M (ratio of convective heat transfer to conductive heat transfer at the base of the fin ($h_b/k_b$)) on the straight fin increase under different nonlinear and international heat generation parameters. Moreover, as the thermogeometric parameter increases, the rate of heat transfer (the convective heat transfer) through the fin increases as the temperature in the fin drops faster. This implies that as convective heat transfer at the base increases (or the base thermal conductivity decreases), M increases and consequently the temperature along the fin, especially at the tip of the fin decreases. The computational results obtained in this study are found to be in good agreement with the standard numerical solutions.

## Model development

Consider a rectangular longitudinal fin of length *l* that is exposed on both faces to a convective environment at temperature, $T_\infty$ and with temperature-dependent heat transfer co-efficient, *h(T),* thermal conductivity, *K(T)* and internal heat generation, $q_{int.}(T)$ shown in Fig.1. Assuming there is no contact resistance where the base of the fin joins the prime surface and the fin thickness is small compared with its height and length, the governing differential equation for the fin as given by:

$$\frac{d}{dx}\left[k(T)\frac{dT}{dx}\right]-\frac{h(T)}{A_{cr}}P(T-T_\infty)+q_{\text{int.}}(T)=0 \tag{1}$$

The boundary conditions are:

$$\begin{aligned} &x=0, \quad T=T_o \\ &x=L, \quad \frac{dT}{dx}=0 \end{aligned} \tag{2}$$

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# The effects of thermal radiation on a reactive hydromagnetic internal heat generating fluid flow through parallel porous plates

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**Abstract**

This study analyses the influence of thermal radiation on an electrically conducting, incompressible and steady flow of a reactive hydromagnetic internal heat generating fluid flowing through a channel between two parallel porous plates; under different chemical kinetics namely: sensitized, Arrhenius and bi-molecular kinetics. The dimensionless governing equations are solved using the modified Adomian decomposition Method (MADM). The velocity and the temperature profiles are investigated for different physical parameters especially the porous medium and thermal radiation parameters. The solutions for the entropy generation rate under different chemical kinetics are obtained using expressions from velocity and temperature profiles and the effects of thermal radiation are also illustrated in physical terms.

**Keywords:**
Chemical kinetics, thermal radiation, reactive fluid, hydromagnetic, internal heat generation and porous medium.

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# The wave scattering analysis of flexible trifurcated waveguide using Mode-Matching approach

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The propagation of waves in a trifurcated waveguide with discrete analogues of hard and flexible outer boundaries is considered. While formulating the related boundary value problem in terms of eigenfunction expansions in different duct regions, the scattering orthogonal and non-orthogonal duct modes are matched using continuity of pressures and velocities across the interface. In this way, the general expressions for the complex amplitudes in all regions are determined in terms of infinite linear algebraic equations. The obtained solution is justified by providing number of analytical and numerical tests; in particular, the relative powers versus frequency regime are displayed graphically. It is worthwhile to mention that the underlying problem provides a standard procedure to model and solve a range of bifurcated and trifurcated waveguide problems with multiple bounding properties of dynamic types include for example, Refs. [1, 2, 3].

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# Turbulence generated by 3D Sparse Multi-Scale Grid

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Flat 2D fractal grids alter turbulence characteristics downstream of the grid as compared to the regular grids with the same blockage ratio and mass inflow rates [1]. This has excited interest in the turbulence community for possible enhanced mixing and related applications. Recently, a new 3D multi-scale grid design has been proposed [2] such that each generation of length scale of grid elements is held in its own frame, in overall co-planar arrangement, Fig. 1. This produces a 'sparse' grid system whereby each generation of grid elements produces a turbulent wake pattern that interacts with the other wake patterns downstream. A critical motivation here is that the effective blockage ratio in the 3D Sparse Grid Turbulence (3DSGT) design is significantly lower than in the flat 2D counterpart – typically the blockage ratio could be reduced from say 20% in 2D down to 4% in the 3DSGT. If this idea can be realized in practice, it could potentially greatly enhance the efficiency of turbulent mixing and transfer processes clearly having many possible applications. Work has begun on the 3DSGT experimentally using Surface Flow Image velocimetry (SFIV) [3] at the European facility in the Max Planck Institute for Dynamics and Self-Organization located in Gottingen, Germany and at the Technical University of Catalonia (UPC) in Spain, and numerically using Direct Numerical Simulation (DNS) at King Fahd University of Petroleum & Minerals (KFUPM) in Saudi Arabia and in University of Warsaw in Poland. DNS is the most useful method to compare the experimental results with, and we are studying different types of codes such as Imcompact3d, and OpenFoam. Many variables will eventually be investigated for optimal mixing conditions. For example, the number of scale generations, the spacing between frames, the size ratio of grid elements, inflow conditions, etc. Fig 2. shows some early analysis of the data, the temporal structure functions up to 5$^{th}$ order, $S_n(t)=<|u(t)-u(0)|^n>$, $n=2,3,4,5$, from velocity time series in air at a point along the channel centreline. We will report in more detail at the time of the conference.

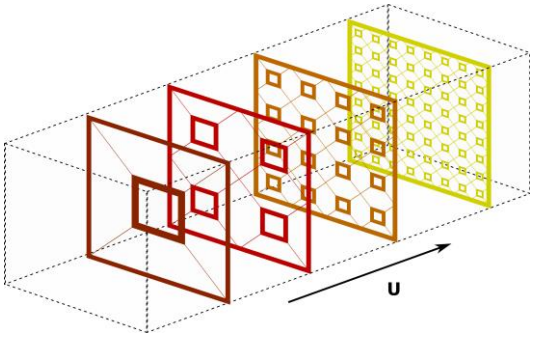


**Figure 1:** Sketch of a 4-generation sparse grid.

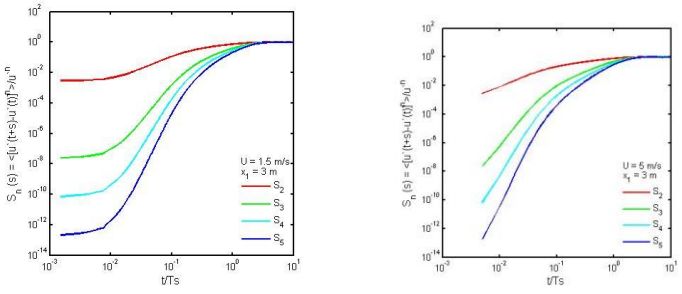


**Figure 2:** Temporal structure functions for mean flow *U = 1.5 m/s* (left), and *5 m/s* (right).

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# CS-MODELING Partial Differential and Integral Equations in Mathematical Modeling

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# A mathematical and numerical framework for bubble meta-screens

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The aim of this paper is to provide a mathematical and numerical framework for the analysis and design of bubble meta-screens. An acoustic meta-screen is a thin sheet with patterned subwavelength structures, which nevertheless has a macroscopic effect on the acoustic wave propagation. In this paper, periodic subwavelength bubbles mounted on a reflective surface (with Dirichlet boundary condition) is considered. It is shown that the structure behaves as an equivalent surface with Neumann boundary condition at the Minnaert resonant frequency which corresponds to a wavelength much greater than the size of the bubbles. Analytical formula for this resonance is derived. Numerical simulations confirm its accuracy and show how it depends on the ratio between the periodicity of the lattice, the size of the bubble, and the distance from the reflective surface. The results of this paper formally explain the super-absorption behavior observed in [1].

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# *A posteriori* error estimates for a multiscale finite element method

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We are interested in the discretization of a diffusion problem with highly oscillating coefficient, by a multi-scale finite element method (MsFEM) treated in ([3],[4], [6] and [7]). The objective of this method is to capture the multi-scale structure of the solution via local basis functions which contain the essential information on small scales. Generally, this method is based on two main ingredients: building multiscale basic functions and variational formulation coupling these functions and providing an accurate approximation of the solution. Multiscale basic functions are designed to capture the characteristics of the multi-scale solution and contain information on small scales.

We develop *a posteriori* estimates for finite element multi-scale method for diffusion problem with a mesh adaptation (see [1], [2] and [5]). The main result consists of building error indicators with respect to both small an large meshes used in this method. We present some numerical experiments which are in good coherency with the results of analysis.

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# Analytic investigation of fingero imbibition phenomena in porous media

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The present paper deals with approximate solution of fingero imbibition phenomena that occurs during secondary oil recovery process in the oil reservoir. There are three steps of oil recovery process, primary, secondary and enhance. The non-linear partial differential equation of the mathematical model has been solved by Optimal homotopy analysis method. For the mathematical modeling, we consider the cylindrical piece of homogeneous porous medium. The graphical representation of the solution is given and has been physically interpreted. The value of convergent control parameter $c_0$ is optimized by reducing the square residual error, so the gives us surety that homotopy series is convergent and so that our solution is consistent. The governing partial differential equation of the problem is given as

$$\frac{\partial S_i}{\partial T} = \frac{\partial}{\partial X}\left(S_i \frac{\partial S_i}{\partial X}\right), \tag{1}$$

subject to the initial and boundary condition

$$\begin{aligned} &S_i(X,0) = \begin{cases} S_{ic}\left(1-e^{-X}\right); 0 < X \leq 1 \\ S_{ic}; X = 0 \end{cases} \\ &S_i(0,T) = S_{ic}; X = 0, T > 0 \\ &S_i(1,T) = f(T); X = 1, T \geq 0 \end{aligned} \tag{2}$$

The equation 1 has been solved by Optimal homotopy analysis method [2] using initial and boundary condition 2. Figure 1 shows that the saturation of injected water is increasing with distance and time increases.

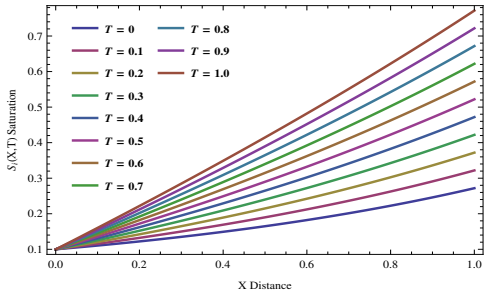


Figure 1: Saturation of injected water $S_i(X,T)$ at different distance $X$ with fix time level $T = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$

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# Common errors in finding conservation laws of differential equations

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Several years ago, two important papers [1, 2] were published on common errors that are often made in investigations of finding exact solutions to nonlinear partial differential equations. These papers were motivated by a large (and still growing) number of publications appearing in the literature in which basic errors were repeated concerning correctness, generality, and novelty of exact solutions, as well as methods for their construction, and proper citation of previous work.

In the past decade, a similar situation has arisen with investigations of finding conservation laws of nonlinear partial differential equations. I will point several common errors that are made in the literature on this topic. The errors deal with generality and novelty of conservation laws, as well as methods for their construction [3], and proper citation of previous work [4].

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# Computational Study of Eventual Periodicity of Forced Oscillations of an Initial-Boundary-Value Problem of the KdV Type Equation

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In this work we consider an initial-boundary-value problem of a KdV type equation on a bounded domain. We demonstrate computationally that if the small amplitude boundary date is periodic of period $\tau$ , then $u(x_0,t)$ at fixed point $x_0$ will eventually becomes time periodic of the same period $\tau$. Several examples are shown by taking various periods. For our numerical solution we have used a collocation technique.

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# Mathematical Model of Binder Distribution During Drying of Lithium-Ion Battery Electrodes

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Electrodes are manufactured by coating a current collector with a slurry mixture, comprised of active material particles, conductive carbon nano-particles, polymer binder and solvent. This mixture is then dried (i.e. the solvent evaporated) by exposure to heat, and sometimes a reduction in pressure. The drying is a crucial step in manufacturing as it can affect the component distribution within the electrode. Phenomena such as binder migration during drying can have negative effects, in the form of poor cell performance or mechanical failure such as electrode peeling and cracking [2, 1]. Despite the importance of the drying process on the microstructure of the product, studies on electrode drying are scarce. As far as the authors are aware, theoretical models detailing the physical mechanisms governing the evolution of the component distributions during drying are as yet unestablished.

We will present a model based on first principles describing the evolution of the binder concentration in the electrode during the drying step of manufacture. Solutions of the model predict that low drying rates lead to a favourable homogenous binder profiles across the electrode film, whereas high drying rates tend to unfavourably accumulate the binder near the evaporation (top) surface. These results show strong qualitative agreement with the experimental data in [1], thereby providing a cogent explanation for why poor electrodes can result from fast drying conditions in practical applications. We will conclude by sketching ideas on how the model could be used to optimize the drying process and by discussing possible extensions of the model.

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# Mathematical Modeling of Double Nonlinear Processes With Source or Absorption

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In last years the nonlinear problems heat conductivity, diffusion, biological population so on, described by the double nonlinear degenerate type differential equations and systems intensively studied by many authors (see [1-9] and references therein). Knowledge of qualitative properties of the solution of the nonlinear differential equations of parabolic type, such as global solvability, estimate and asymptotic of solution, condition of arising blow up solution is very important for the computing purposes depending on value of numerical parameters of the considered problems.

In this talk we demonstrate the possibilities of the self-similar, approximately self-similar approaches to the studying of properties of double nonlinear reaction-diffusion systems with source. An influence of parameters of the reaction-diffusion systems to an evolution of the process is investigated. The algorithm for establishing the Fujita type and the second critical exponents is offered. Based on this algorithm a global solvability of the Cauchy problem for a slowly and a fast diffusion cases is established. Main member of an asymptotic behavior of a self-similar solution is obtained. It is proved that there exist some values of parameters when the effect of finite velocity of perturbations, localization of solution, blow up have place. Based on qualitative properties of solutions and an establishing sub and sup solution the numerical analysis of solutions is made. The problem of the finding an appropriable initial approximation of solutions depending on value of the numerical parameters is solved. Results of the numerical analysis is discussed.

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# Modeling and Simulation of Reaction-Transport Interactions Using Fractional Anomalous Diffusion

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Reaction-Transport interactions are commonly used to describe chemical and biotechnological industrial processes [1,2]. For instance, tubular chemical reactors, reactive distillation, catalyst particles, upflow anaerobic sludge blanket reactors, etc. Mass diffusion transport is usually modeled by the continuity equation and the Fick's first law. However, Fick diffusion describes infinite velocities of propagation, which is unrealistic. Thus, to avoid the unphysical effects, produced by traditional diffusion, the use of anomalous diffusion to describe mass diffusion has been proposed [3-5].

For a description of anomalous diffusion phenomena, models based on the Cattaneo's diffusion models with entire or fractional order have been proposed [6,7]. In particular, the fractional Cattaneo's diffusion model has been validated experimentally, however it has poorly studied for modeling and simulation of reaction-transport interactions in industrial problems.

In this work, we present a systematic overview of the approach and solution of reaction-transport models considering anomalous transport mechanisms. As a case study, the dynamics of a catalytic pellet using fractional Cattaneo-type generalized reaction-diffusion models is proposed. For the numerical solution, an implicit method is proposed using Grünwald-Letnikov finite difference schemes [8]. The results show the effect of the relaxation time and the fractional derivative order, on the concentration profile and the effectiveness factor dynamics, concluding that the adjustment of these parameters allows adjustment of the profiles where anomalous transport mechanisms are relevant.

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# $MOL^T$ Based Fast High-Order Three Dimensional A-Stable Scheme for Wave Propagation

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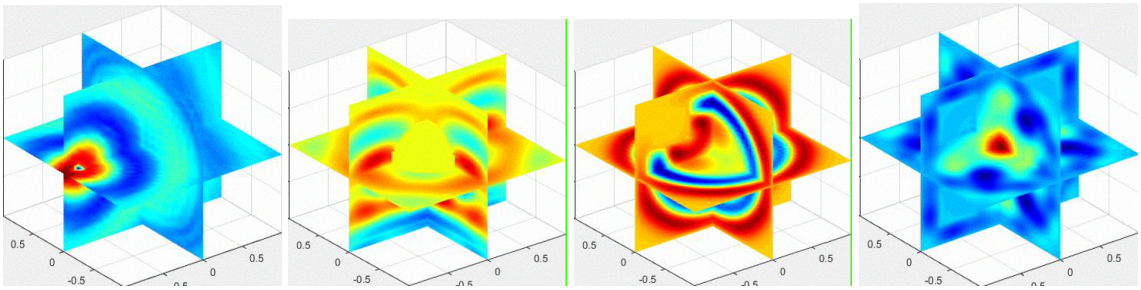
We present a fast (linear-time), high-order, multi-dimensional, A-stable implicit wave solver applicable for electromagnetic (EM) problems, specifically targeting plasma science. This approach uses a Method Of Lines Transpose ($MOL^T$) formulation combined with an Alternating Direction Implicit (ADI) scheme. In this scheme, a PDE is first discretized in time, and then the resulting boundary-value problems are solved using a Green's function method [1]. In particular, inverse of the resulting modified Helmholtz operator is analytically constructed and evaluated efficiently using an $O(N)$ recursive fast convolution algorithm. Extension to multi-dimensions is formed using an ADI scheme, and each line is solved independently. Complex geometries are handled with an embedded boundary method (see [2] for second order accurate 2D scheme). In this work, we propose a higher order 3D scheme which is able to deal with complicated geometries using an embedded boundary method. The high order scheme is achieved by utilizing a Lax-Wendroff approach to exchange time derivatives with spatial derivatives using even powers of the Laplacian [3]. The scheme is successfully evaluated using several 3D test problems and it's ability to handle complex geometries is verified using simulations of scattering by PEC spheres (Figure 1).



(a) (b) (c) (d)

Figure 1: 3D wave propagation a) of a point source, with b) a PEC sphere placed at the center, and of a Gaussian pulse with b) a cubic patch placed at the left top corner, and c) 4 cubic patches placed at the four corners along *xz* plane.

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# Multi-Scale Model Formulation of a Porous Medium Biofilm Reactor and the Effect of Planktonic Bacteria and Attachment on Reactor Performance.

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The objective of this study is to derive a multi-scale model for biofilm formation in a porous medium reactor. The starting point is the traditional mesoscopic one-dimensional Wanner-Gujer biofilm model. Mesoscopic processes included in the model are hydrodynamics and transport of substrates in the reactor, biofilm and planktonic bacteria growth in the pore space through consumption of a single, non-reproducing growth limiting substrate, attachment of planktonic cells to the biofilm, detachment of biofilm cells, and cell lysis. Using a similar process as described in [1], the mesoscopic equations are up-scaled from the biofilm scale to the reactor scale (macroscale), yielding a stiff system of quasilinear hyperbolic balance laws.

We study the macroscopic system of partial differential equations (PDE) numerically using the Uniformly accurate Central Scheme of Order 2 (UCS2) proposed in [2]. Through evaluating the coefficient functions of the system, we calculate the flux of substrate into the biofilm as the solution to a two-point boundary value problem describing the substrate concentration in the biofilm layer.

In this study we investigate and compare two different mesoscopic flux functions and their effect on the solution to the macroscopic system. The first function is a linear approximation of the flux in a substrate limiting regime, while the second function is the more classical Monod function. The role of planktonic bacteria and the effect mesoscopic attachment has on macroscopic reactor performance is also investigated.

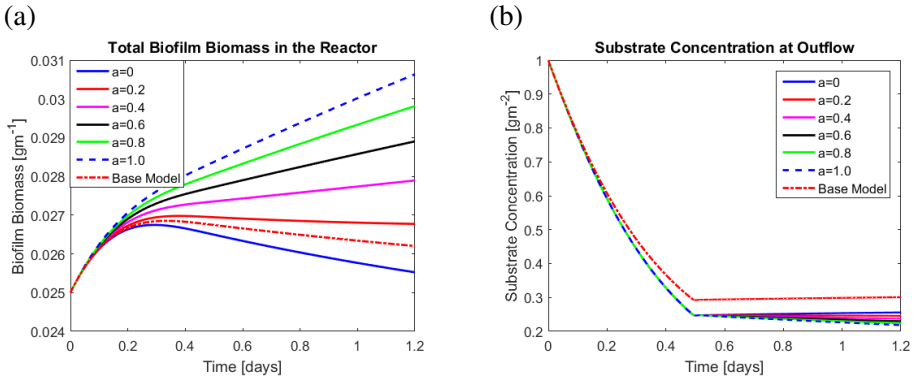


Figure 1: Linear approximation of biofilm flux and the effect of variable attachment rates on **(a):** total biomass in the reactor and **(b):** degradation of substrate concentration at outflow.

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# Numerical Modeling of Hydraulically Fractured Shale Gas Reservoirs

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Shale gas reservoirs are characterized by their low permeability and various flow regimes that occur due to the complex geology of the rocks. Gas residuals are trapped in these fractures over very large areas, and it can be released from fractures with the use hydraulic fracturing techniques. We have attempted to numerically model the fluid flow through hydraulically fractured shale gas reservoirs. In this scenario, we discuss the ways to discretize the domain, especially near the surface of the matrix, where the rapid changes in the fluid pressure occur. The governing equations are solved using control volume finite element formulation on a simple (idealized) fracture pattern, and the results are illustrated.

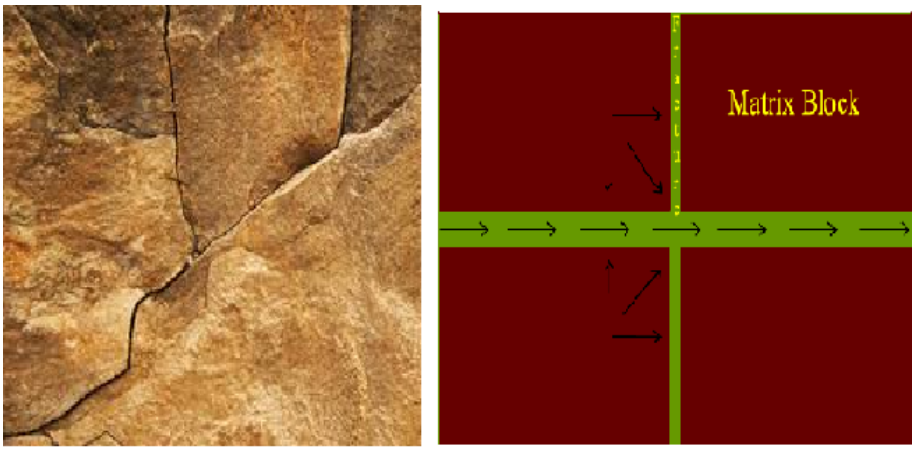


Figure 1: A fractured shale gas reservoir filled with hydrocarbon residuals.

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# Numerical Simulations of Reaction-diffusion Equations Modeling Prey-predator Interaction with Delay

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To model biological systems one often uses ordinary and partial differential equations. These systems can be quite good at approximating observed behavior, but they suffer from the downfall of containing many parameters, often signifying quantities which cannot be determined experimentally. For the better understanding of complicated phenomena, the delay differential equation approach to model such phenomena is becoming more and more essential to capture the rich variety of dynamics observed in natural systems. In this study, we investigated numerically the influence of delay on the dynamics of reaction-diffusion equations modeling prey-predator interaction using finite difference scheme subject to appropriate initial and boundary conditions (Refs. [1-3]). We first consider the prey-predator with Hollinq type II functional response where the growth of prey is assumed to be logistic in the sense of predator in one-dimensional space. The effect of delay was investigated with the help of simulations and is compared with the model equation without delay. The proposed method is then extended to two-dimensional space.

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# Numerical Solutions of Boundary-Contact Problems to the Thermal Diffusion Models of Non-Classical Theory Coupled-Elasticity

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Many methods in the theory of non-classical thermo elasticity require to the solution of boundary-contact problems (BCPs). A great attention is to construction of solutions in the form that admit efficient numerical evaluation [1].

In this work numerical approximation to the solution of BCPs for two-dimensional generalized coupled thermo elastic diffusion materials [2] with thermal and diffusion relaxation times has been developed in the Green-Lindsay formulation. In particular the problem is investigated for isotropic inhomogeneous finite and infinite domains with inclusion of several elastic materials in assumptions that surfaces are sufficiently smooth and solutions satisfy the radiation conditions in infinite.

Numerical results have been obtained for boundary-contact conditions when the couple-stresses components, displacement components, rotation, heat flux and temperature, concentration and chemical potential are represented on the surfaces of Holder class.

The tools applied in this development are based on singular integral equations, Laplace transform, the potential method, Green's Tensors and the generalized Fourier series analysis.

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# On global properties of Gowdy spacetimes in scalar-tensor theory

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Recent results show that standard singularity theorem that holds when an energy condition is applied in general relativity also holds when that energy condition is applied to the Bakry-Emery-Ricci tensor which naturally arises in the scalar-tensor theory of gravity. The theory is one of the generalized theories of gravitation and is a low energy effective superstring theory. Thus it is important to investigate global behavior of solutions to the gravitational field equations in the theory. We study the global properties of the Gowdy metrics generated by Cauchy data on $T^3$ in the Brans-Dicke theory which is one of the scalar-tensor theory of gravity. We show that the past boundaries of the maximal Cauchy developments of Gowdy initial data sets are asymptotically velocity-terms dominated singularities. The Kretschmann scalar blows up on the boundary. Thus the maximal Cauchy development cannot extend beyond the boundary and our result shows that the validity of the strong cosmic censorship conjecture.

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# On the breach of conservation laws in fragmentation processes

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In this presentation, we review conservation laws in fragmentation equations and discuss scenarios leading to the breach of conservativeness. Semigroup theory will be used to investigate the interfacial dynamics of the corresponding evolution equations [1]. In particular, Laplace transforms will be considered to solve a class of fragmental integro-differential equations and study their asymptotic behavior [2].

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# Rogue waves in the Generalized Davey-Stewartson System

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Rogue waves are rare uncertainly emerging localized waves with large amplitudes. They occur in many nonlinear wave phenomena, such as the water, optical and acoustic waves. In this study, we consider dynamics of rogue waves in the generalized Davey-Stewartson (GDS) system, given by

$$\begin{aligned} iA_t &= \gamma_{11}A_{xx} + \gamma_{12}A_{xy} + \gamma_{22}A_{yy} + \chi|A|^2A + A\left(\beta_1\frac{\partial}{\partial x} + \beta_2\frac{\partial}{\partial y}\right)Q, \\ \alpha_{11}Q_{xx} + \alpha_{22}Q_{yy} &= -2\left(\beta_1\frac{\partial}{\partial x} + \beta_2\frac{\partial}{\partial y}\right)|A|^2. \end{aligned} \tag{1}$$

The GDS system is obtained for the weakly nonlinear modulation of a wave originated by the interaction between a long wave-length acoustic mode and a high frequency mode in [1]. Thus the real mode $Q$ represents a mean motion induced by the oscillatory wave packet, which has the complex amplitude $A$. System (1) for $(\gamma_{12}, \beta_2) = (0, 0)$ reduces to the Davey-Stewartson (DS) system. On the other hand, rogue waves in DS are also derived by the Hirota's method [2, 3]. We follow a similar approach and find line-, multi- and higher order rogue waves in the GDS system (1). It is also obsevered that there are different features among these rouge waves.

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# Self-Similar Solutions for a Degenerate Parabolic System Not in Divergence Form

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Consider the parabolic system in non-divergence form with Cauchy conditions

$$|x|^s \frac{\partial u}{\partial t} = v^{m_1} \nabla\left(\left|\nabla u^k\right|^{p-2} \nabla u^n\right),\ |x|^s \frac{\partial v}{\partial t} = u^{m_2} \nabla\left(\left|\nabla v^k\right|^{p-2} \nabla v^n\right),\quad t>0,\ x \in R^N \tag{1}$$

$$u|_{t=0} = u_0(x) \geq 0,\quad v|_{t=0} = v_0(x) \geq 0,\quad x \in R^N \tag{2}$$

where $s, k, p, n, m_1, m_2$ are positive constants.

Non-divergence form equations and system equations comparing with the classical divergence form equations are more close to the actual circumstances in some cases. For example, for the biological species, the diffusion of divergence form implies that the species is able to move to all locations within its environment with equal probability, but if we consider this problem with the objective conditions, the population density will affects the rate of diffusion, so a kind of 'biased' diffusion equation will be more realistic, for the non-divergence form diffusion. The diffusion rate is regulated by population densities that is increasing for large populations and decreasing for small populations, see for [1-7].

In this abstract asymptotic behavior of self-similar solutions for a degenerate parabolic system not in divergence form (1) for slow and the fast diffusion cases depending on value of the numerical parameters are studied. The property a finite speed of a perturbation of distribution to the Cauchy problem for a nonlinear parabolic system not in divergence form based on comparison method are established. It is shown that coefficients of main member of asymptotic solution satisfy to some system of nonlinear algebraic equations. It is found the Zeldovich-Barenblatt type solution to the parabolic system. On the basis of this asymptotic of solutions, suitable initial approximations are offered in the iterative process for the slow and fast diffusion cases, depending on the values of the numeric parameters.

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# Strip-saturation model for mode-III semi-permeable collinear cracks weakening a piezoelectric strip

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## Abstract

A mathematical strip-saturation model solution for transversely isotropic piezoelectric strip, weakened by transversely oriented and symmetrically situated two mode-III collinear cracks, is obtained. The strip is assumed electrically poled in the direction perpendicular to the length of the cracks. The piezoelectric strip being prescribed out-of-plane shear stress $\tau_0$ and in-plane electric-displacement $D_0$. Consequently, under the combined electro-mechanical loadings, cracks open in self-similar fashion and form saturation zones ahead of each tip of the cracks. The piezoelectric ceramic being brittle, the developed mechanical zone is assumed to be of negligible length, hence ignored. The developed saturation zone is prescribed in-plane normal cohesive polarization limit electric-displacement $,D_s$. The crack surfaces are assumed to be traction free and cracks are electrically semi-permeable.

The analytical solution of the mathematical model framed of above problem solved using Fourier series method. Which reduces the problem to two sets of triple series equations. Each of the triple series equations set is further reduced to a singular integral equation of Cauchy kernel type using integral equation technique.

Closed-form analytic expressions are derived for length of developed saturation zones and fracture parameters {crack sliding displacement (CSD), crack opening potential drop (COP), field intensity factors (IFs), local energy release rate (LERR) and global energy release rate (GERR)}.

The above study is presented for all electric crack-face boundary conditions: impermeable, permeable and semi-permeable.

A case study is presented for different poled $BaTiO_3$, PZT-5H, PZT-6B, PZT-7A piezoelectric materials. The influence of inter-crack distance, electric crack-face boundary conditions, piezoelectric material constants and prescribed electro-mechanical loadings on CSD, COP, IFs, LERR and GERR are presented graphically and compared.

From the numerical results, it is seen that cracks open more for small value of inter-crack distance and as the separation between two cracks increases, the value of fracture parameters decreases, indicates that the material would be more stable when the cracks are apart from each other.

Also, the value of fracture parameters are maximum for impermeable case and minimum for permeable case. For semi-permeable case, these lie between impermeable and permeable cases. This indicates that the electric permittivity of medium inside the crack can not be ignored.

Finally, all the graphical variations conclude that proposed model is capable to crack arrest under small-scale electric yielding.

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# The Preserving Neutron Flux Properties Discrete Scheme for Multi-media Time-dependent Neutron Transport Equations

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There exit numerical solution oscillation and negative flux for typical discrete scheme when solving multi-group multi-media sophisticated time-dependent neutron transport equations which brings difficulty for mathematics and physics analysis. In this paper, the numerical solution oscillation for sophisticated problem is investigated. The influence of time discrete scheme and space discrete scheme on this oscillating phenomenon is analyzed for neutron transport equations. In addition, the preserving positive neutron transport scheme (PPLD) is studied. The new scheme can take 0 order moment and 1 order moment of the neutron transport equation.

Numerical experiments show that second-order time evolution scheme and linear discontinuous finite element method yield more accurate results and provide very smooth physical quantity curves. Based on the non-oscillation scheme, the positive scheme gives the non-negative neutron angular flux. These preserving physical properties neutron transport schemes maintain the smooth of neutron multiplication constant and positivity of neutron flux.

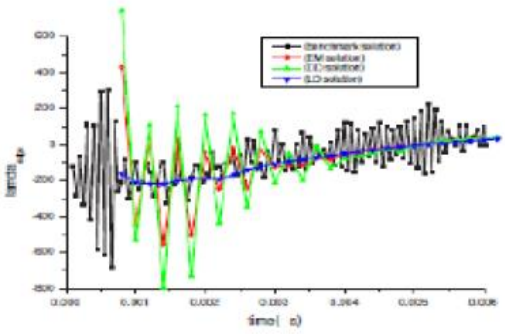

Figure 1: J for mutigroup problem

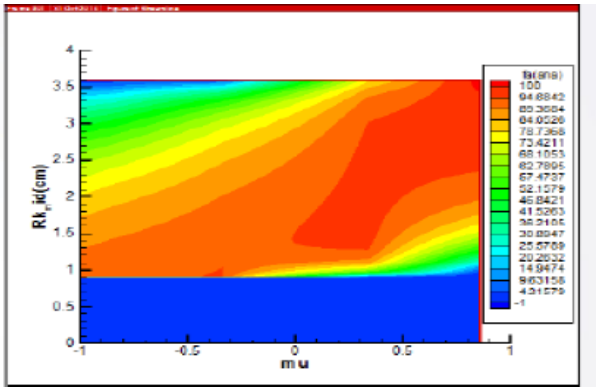


Figure 2: flux for PPLD method
(the maximal value is 102.732, the minimal value is 0)

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# Tug of war games and PDES on graphs with applications in Image processing and Machine Learning

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Game theoretic stochastic or deterministic methods have recently emerged as a novel approach to study and to approximate various non-linear Partial Differential Equations (PDEs). In particular Tug-of-War Games (TOG) related to the $\infty$-Laplacian or to the $p$-Laplacian have attracted a lot of attention. They were first introduced by Peres, Schramm, Sheffiel, and Wilson in [1]. It is now used in many works to study the existence or the regularity of solutions for many PDEs. Many of these games generally are formulated as well-known statistical functionals such as *mean*; *min*, or *max* operators. They are interpreted as a discrete approximation of the underlying PDE and solving the latter leads to taking a suitable limit of the solution of the discrete game.

Recently, there is a high interest in adapting classical signal processing tools on graphs and networks such as wavelets or PDEs [2]. The demand for such methods is motivated by existing and potential future applications, such as in machine learning and mathematical image processing. Indeed, any kind of data can be represented by a graph in an abstract form in which the vertices are associated to the data and the edges correspond to relationships within data.

In this paper, we consider a general Dynamic Programming Equation that encompasses many versions Tug-of-War Games arising in the discrete game theoretic interpretation for various non-linear PDEs including $\infty$-Laplacian, game $p$-Laplacian and Hamilton-Jacobi related equations. We show that under our framework of Partial difference Equations (PdEs) [2], these discrete games coincide with PDEs on particular Euclidean graphs.

The same PDEs on weighted graph of arbitrary topology lead to non-local statistical functionals, including well-known non-local means, non-local dilation, and non-local erosion operators. We interpret them as non-local Tug-of-War Games and we show their connection to non-local PDEs on Euclidean graphs.

This paper unfolds as follows: first, we briefly introduce several discrete games, their related PDEs, and the previously proposed Partial difference Equations (PdE) framework. Then, we naturally extend these games to non-local forms, and illustrate some interpolation problems on image and point cloud processing.

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# CS-POST AMMCS-2017 Poster Session

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# A Model for the Prediction of the Growth and Activity of a Lung Tumor

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In our work, we are interested to study model of growth of a non-vascularized tumor in the lung of [1]which is a simplification of the spatial model of [2]. This model aims to compute the tumor volume denoted V. we consider the problem of the modelization of a tumor growth. We study two models in this contest, the first concerns the growth of a tumor non subjected to a treatment (1), and the second concerns a tumor subjected to a treatment(2) .

$$\begin{cases} \frac{dV}{dt} = \gamma PV \\ \frac{dP}{dt} = \gamma P(1-P) - (1-\gamma)P \\ \frac{dC}{dt} = (1-C)(\frac{V}{V_0})^{\frac{2}{3}} - \alpha PC \\ \gamma = \frac{1+tanh(R(C-C_{hyp}))}{2}. \end{cases} \tag{1}$$

To model the addition of a treatement of chemotherapy, we adid to the equation of P , witch is the number of cells in the proliferation, a term that decreases in time to simulate chemotherapy. We will consider chemotherapy consists of several injections. In this work, we use another form of this term giving as follows :

$$\begin{cases} \frac{dV}{dt} = \gamma PV, \\ \frac{dP}{dt} = \gamma P(1-P) - (1-\gamma)P - \beta \sum_{i=0}^{2} f_i 1_{t>t_i} \frac{1}{\lambda(t-t_i)+1} P, \\ \frac{dC}{dt} = (1-C)(\frac{V}{V_0})^{\frac{2}{3}} - \alpha PC, \\ \gamma = \frac{1+tanh(R(C-C_{hyp}))}{2}. \end{cases} \tag{2}$$

We also present some numerical results. From the model (1), We illustrate the effect of these factors by a simulation study. In the two cases of the growth of the tumor, with or without treatment, we take diffrent values of $C_{hyp}$ and $\beta$, and we compare the graphs of V and/ or P that we obtain, in order to highlight the effect of $C_{hyp}$ and then that of $\gamma$ and $\beta$.

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# A New Discrete model for the Simulation of a non-linear Differential Equation Arising from the Dynamics of the Tsunami Tidal Waves

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This work present new Discrete models for the simulation of a Tsunami Tidal waves. We developed a new finite difference scheme using a combination of dynamically normalized denominator function , non-local approximation and an exponential interpolating function.
A lot of earlier and present study of the Tsunami Tidal waves employ the same phenomena.
Though some earlier modelers assumed Tsunamis to be linear, long gravity waves at single frequencies some other models that have proven very useful has employed non-linear views
The model under study is based on the estimation of tsunami run-up heights at different points along the coastline. The Tsunami Model under study is given by $\left(\frac{dy}{dx}\right)^2 = y^2(4-2y); y(x) > 0$ is the height of the wave expressed as a function of its position relative to a point off-sore.
Such are the works of : Wei, Y., E. etal (2008) ,Mofjeld, H.O. (2009). Some research works based on numerical models for the simulation Tsunami Tidal waves include the following: Mader C.L.*, 1988.*, Ivanov B.A. & Artemieva N.A.*, 2002.* Earlier Finite Difference schemes for this model produces qualitative properties like monotonicity of solutions, monotone dependence on initial values and local stability . We constructed new NonStandard schemes with the same properties with far lower absolute error of deviation **.** We also create a new Discrete model using interpolation of $y(x) = a_0 + a_1 e^{\alpha x} + a_2 e^{-\beta x}$ by assuming a solution consisting of both decaying and increasing phenomena in which can become self balancing or tilted substantially into either the decay or growth component depending on the value of some parameters $\alpha$ *and* $\beta$ .from where we obtained **locally stable , convergent and consistent** Hybrid NonStandard schemes with absolute error of deviation **below 0.0001. Thus** we found the new discrete models significant based on the substantial amount of improvement in cumulative and relative absolute error of deviation from the known analytic solution . The schemes have been tested in a numerical experiment which produced some interesting 3D graphs. This work has shown that the combination of Nonstandard method (Mickens R. E (1994) and Anguelov R., Lubuma J.M.S. (2003))and interpolation methods can provide a better scheme for Nonlinear Ordinary Differential Equation

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# A New Similarity Method for Searching Organic Chemical Structures

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Today, setting up a platform to produce, represent, and share information on various aspects of organic chemistry research such as cheminformatics, data analysis, and synthetic design is still a very important issue. How to search and represent organic chemical structures remains challenging research topics. Several research groups have addressed these two topics and some practical solutions have been proposed.

How to measure similarity between molecules is a fundamental problem in cheminformatics. The similar molecules seem to have similar chemical and biological properties. The concept of molecular similarity plays an important role in the exploration of molecular data analysis. Several methods have been demonstrated to define molecular similarity. However none of them have been shown with accurate results for organic chemical structures. In this research, we propose a new similarity method which is based on organic compounds atom structural features for analyzing similarity between molecules. In particular, our proposed method is based on the comparison of the bonding structure of atoms on comparable organic molecules, including special features such as organic compounds chirality and stereoisomerism.

Key words: structural search, cheminformatics, data analysis.

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# Convergence of the Regularized Sinc Collocation Method Applied to Fredholm Integral Equation

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Many problems in applied mathematics and engineering can be formulated as Fredholm integral equations of the first kind:

$$Kf(x) = \int_a^b k(x,y)f(y)dy = g(x), \tag{1}$$

where the kernel $k(.,.)$ and the right-hand side $g$ are smooth real-valued functions.

The determination of the solution $f$ of iefk is an ill-posed problem in the sense of Hadamard; in the sense that the solution (if it exists) does not depend continuously on the data.

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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# Fractional Order Total Variation Based Model for Multiplicative Noise Removal

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In this paper we proposed a new fractional order total variation (FOTV) based model via weighted statistic for restoration of images corrupted with multiplicative noise. Explicit time marching scheme is applied to find the solution of the corresponding Euler-Lagrange partial differential equation. Experimental results demonstrate that our proposed methodology improves the visual quality of the restored images as well as increase the peak signal to noise ratio (PSNR) over other existed methods.
**Key points**: Total Variation, Euler-Lagrange Equation, Discrete Fractional Order Differences, Speckle Noise, Image Restoration.

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# Mathematical Kinematic Modelling of a New 3DOF micro-CMM Parallel Manipulator

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In this work, a mathematical kinematic model is developed for a new design of micro coordinate measurement machine (micro-CMM). The machine is proposed for high precision and high accuracy micron scale measurements of three-dimensional objects. The mechanism of the machine is based on 3 degrees of freedom (3DOF) parallel manipulator, where the end effector of this micro-CMM carries a contact touch probe. This design is intended to achieve submicron accuracy for a work envelope of at least (100x100x100) mm. In this paper, the coordinate system of the prototype machine was developed then its kinematic, measurement and error models are derived.

The kinematic position model was able to explicitly define the coordinate of the probe in x, y and z directions, this was validated using a conventional CMM. Results show that an average difference of less than 0.5 mm over a set of 30 points is achieved. This result of the micro-CMM demonstrator measurements falls within the error budget of approximately 0.75 mm estimated by the proposed analytical error model.

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# Modeling and Simulation of Phenol Degradation in a Cascade Photoreactor

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Strict pollution control legislation in the world has led to research for the development of new and efficient water treatment technologies [1]. According to published studies, advanced oxidation processes (POAs) have demonstrated high efficiency, where waste oxidation can increase levels of biodegradability by lowering the initial organic load [2,3]. POAs are attractive technologies to destroy organic pollutants because they are mainly based on the generation of hydroxyl radicals, very reactive species, which cause the destruction of the organic pollutant due to its high oxidizing.

Heterogeneous photocatalysis (HP) degradation is one of the leading POAs technologies used for contaminant degradation in several kinds of wastewaters. HP consists in the adsorption of radiant energy by a photocatalyst [3,4]. At the interfacial region between the excited solid and the wastewater solution reactions take place for the degradation of contaminants. Some drawbacks of HP are low quantum efficiency, the design of the photoreactor, the recovery, reuse and deactivation of the of catalyst, and the generation of toxic intermediates [3-5].

To improve the understanding and performance of HP is of paramount importance the development of mathematical models [5,6]. In the present work, we have developed a mathematical modeling of phenol photodegradation in a cascade type photoreactor using $Fe_2(SO_4)_3$ as a catalyst. The proposed model includes the incident UV radiation (absorption-dispersion of photons within the reaction space), and reaction kinetics. The proposed approach involves the use of the Monte Carlo method to model the Radiation Transfer Equation (RTE) inside the photoreactor, method used to determine the irradiation time of the photocatalyst in the photoreactor and finally to predict the photocatalytic efficiency in general.

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# Numerical Simulation of Tracer Tests in Porous Media Based on a Green's Functions Formulation

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Tracer transport in porous media has been a topic of extensive research over the last few decades. Tracer test have been used to measure porous media parameters like longitudinal dispersivity, effective porosity, solute sorption, rate of solute degradation, non-aqueous phase liquid (NAPL) saturation, and rate of mass transfer into zones of immobile water [1-3].

The tracer test consists of an injection of a prepared solution (containing the tracer and/or partitioning compounds) into a fractured media, followed by the extraction of the solution. Desired properties or parameters are obtained through the interpretation of concentration versus time breakthrough data collected during the extraction stage [1,2].

Experimental tracer tests are expensive, and the desired results are not always obtained. Thus, to predict the behavior of the tracer in the porous media mathematical models of different levels of complexity have been proposed. A practical model invokes the dual-porosity conceptualization of fractured rocks, which is based on considering that water flows in parallel fractures, which are separated by slabs of porous rock matrix containing stagnant pore fluid [2,4]. Double porosity type models have been solved using the Laplace transform, implicit differences methods and software programs based on finite element methods [2-5]. In this work, we propose the use of numerical schemes based on Green's function formulations [6]. The mathematical structure of the proposed scheme allows identifying the individual contributions of the reaction-transport system, i.e., the transport phenomena, chemical reactions, boundary conditions and dynamic accumulation effects. To illustrate the properties of integral formulations, two general case studies of tracer test models in fractured reservoirs are considered, involving reaction-diffusion and reaction-diffusion-convection interactions. The obtained results indicate that the numerical scheme proposed is systematic and easy to apply in tracer test models, improve numerical approximations up to 3 orders of magnitude compared with classical finite difference schemes, and significantly reduce computation times.

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# Numerical Simulation of Ultrasound-Driven Bubble Motion on a Wall

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Bubble motion in an ultrasonic field is of great interest in various applications including ultrasound cleaning, hydrodynamic erosion and medical treatment. For its practical applications, a fundamental understanding and prediction of the bubble motion is essentially important. In this work, we focus on ultrasound-driven bubble motion on a wall.

Numerical simulations of compressible bubble motion were performed using a level-set (LS) method [1-2], a front-tracking method [3] and the volume-of-fluid (VOF) method [4]. The interface tracking methods were coupled to the ghost fluid method (GFM) [1], which is a numerical technique for efficiently implementing the matching conditions at the interface. However, the computations were not extended to the compressible bubble motion on a wall.

In this work, the LS method is extended to include the effect of compressibility of bubble and liquid and the effect of contact angle at the liquid-gas-solid contact line. The conservation equations of mass and momentum are solved by incorporating the GFM, which is modified for the compressible two-phase flows with large density difference. The semi-implicit pressure correction method [2] is also incorporated into the LS method for avoiding the serous time step restriction in low Mach number (or near incompressible) flows.

The numerical method is applied to investigate the effects of ultrasonic amplitude, bubble size and contact angle on the bubble motion. A spherical bubble of 5-10 $\mu m$ radius is placed on a wall while the ultrasound of 0.725 MHz frequency and 0.2-0.4 atm amplitude is imposed through a liquid water layer of 0.53 mm thickness. The numerical results show that the bubble motion and the associated pressure pulsing at the wall are significantly affected by the contact angle as well as the ultrasonic amplitude and bubble size, as plotted in Figure 1.

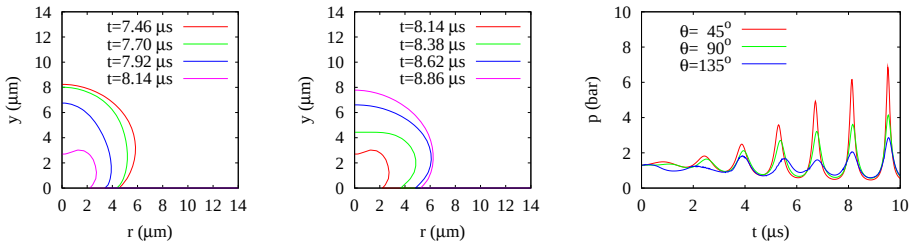


Figure 1: Ultrasound-driven bubble motion at $\theta = 45^o$ and the effect of contact angle on the wall pressure.

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# Quantum mechanical free energy profile of the water dimer over a broad range of temperatures

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Free energy calculations provide a great deal of information about a system but are often computationally intractable for all but the simplest of systems. Traditional molecular dynamics simulations are governed by the Boltzmann distribution but the Boltzmann distribution poorly samples areas of phase space that may be separated by large potential wells. For classical simulations, various enhanced sampling techniques have been developed in order to improve the sampling efficiency. However, there are many situations where nuclear quantum effects play a significant role in these types of simulations. Previous work has studied the combination of path integral simulations in conjunction with umbrella sampling where the biasing potential has been applied to the centroid of the path as opposed to the individual path integral beads.[1, 2, 3] In the present work, we have prescribed a methodology wherein the umbrella sampling biasing potential is only applied to a single bead such that

$$Z_{\mathrm{d}}^{\mathrm{PQC}} = \mathrm{Tr}\left[e^{-\beta\left(\hat{K}+\hat{V}\right)}e^{-\beta\hat{V}_{\mathrm{bias}}}\right] \tag{1}$$

$$= \lim_{P\to\infty}\int \mathrm{d}R_1\ldots\mathrm{d}R_P\prod_{i=1}^{P}\rho_\tau(R_i,R_{i+1})\times e^{-\beta V_{\mathrm{bias}}(R_1)}\ , \tag{2}$$

where $\rho_\tau$ is the high temperature density matrix used in the path integral evaluation and $V_{\mathrm{bias}}(R_1)$ is the umbrella sampling biasing potential as a function of only the first bead in the path integral. We have validated this definition against a Lennard-Jones $Ar_2$ benchmark system that we may solve for exactly before applying it further to the more complicated water dimer system over a broad temperature range. We obtained free energy profiles which were utilized in the calculation of second virial coefficients for the high temperature regime as well as the free energy difference between separated monomers and dimer in the low temperature regime. Comparisons to experimental values for both the second virial coefficient at reasonable temperatures and dissociation energy of the dimer in the ground state are made. [4, 5, 6, 7]

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# Spatial Correlation as an Early Warning Signal of a Critical Transition in a Multiplex Disease-Behaviour Network

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Early warning signals of critical transitions are a widely studied phenomenon because they can provide the ability to quantify a system's proximity to a tipping point to a new and contrasting dynamical regime. However, this effect has been little studied in the context of the complex interactions between disease dynamics and vaccinating behaviour. Our objective was to determine whether critical slowing down (CSD) occurs in a multiplex network that captures opinion propagation on one network layer, and disease spread on a second network layer. We parameterized a network simulation model to represent a hypothetical self-limiting, acute, vaccine-preventable infection with short-lived natural immunity. We tested five different network types: random, lattice, small-world, scale-free, and an empirically derived network. For the first four network types, the model exhibits a critical transition as perceived vaccine risk moves beyond a tipping point, from full vaccine acceptance and disease elimination to full vaccine refusal and disease endemicity. This critical transition is preceded by an increase in the spatial correlation in non-vaccinator opinions beginning well before the bifurcation point, indicating CSD. The early warning signals occur across a wide range of parameter values. However, the more gradual transition exhibited in the empirically-derived network underscores the need for further research before it can be determined whether trends in spatial correlation in real-world social networks represent critical slowing down. The potential upside of having this monitoring ability suggests that this is a worthwhile area for further research.

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