# AMMCS 2019 INTERNATIONAL CONFERENCE



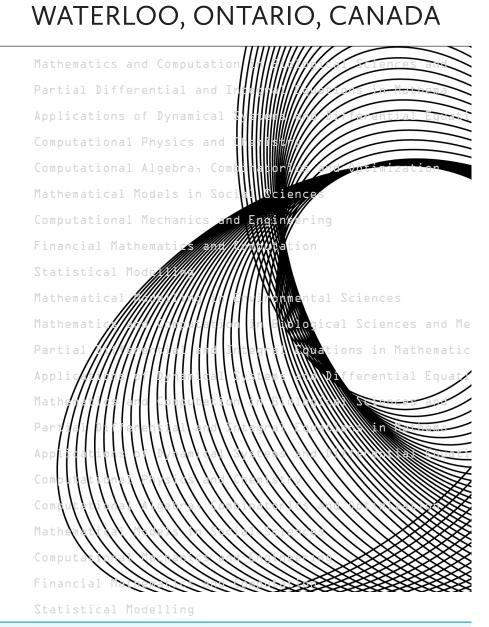
# **AUGUST 18-23**

# BOOK OF ABSTRACTS

### **General Chairs**

Marc Kilgour Roderick Melnik Sunny Wang





# The AMMCS 2019 Conference Book of Abstracts

Waterloo, Ontario, Canada

August 18–23, 2019

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SS-GTMDS	Geometric and Topological Methods in Data Science
SS-IDAHDMD	Interdisciplinary Data Analysis of High-Dimensional Multimodal Data
SS-MF	Mathematical Finance
SS-MMNN	Mathematical Models for Nanoscience and Nanotechnology
SS-MMLSM	Mathematical Modelling in Life Sciences and Medicine
SS-MSWID	The Mathematics and Statistics of Wealth and Income Distributions
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CODE	TITLE
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CS-CACO	Computational Algebra, Combinatorics, and Optimization
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CS-DSDE	Applications of Dynamical Systems and Differential Equations
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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-2019 Poster Session

## Lectures

# **Plenary Lectures**

### **Extreme Democracy**

### Ariel Procaccia, Carnegie Mellon University

Abstract: I will present the 'virtual democracy' framework for the design of ethical AI. In a nutshell, the framework consists of three steps: first, collect preferences from voters on example dilemmas; second, learn models of their preferences, which generalize to any (previously unseen) dilemma; and third, at runtime, predict the voters' preferences on the current dilemma, and aggregate these virtual 'votes' using a voting rule to reach a decision. I will focus on two instantiations of this approach: a proof-of concept system that decides ethical dilemmas potentially faced by autonomous vehicles, and a decision support tool designed to help a Pittsburgh-based nonprofit allocate food donations to recipient organizations. These projects bridge AI, social choice theory, statistics, and human-computer interaction; I will discuss challenges in all of these areas.

### Simple Approaches to Complex Data with Lyme Application

### Deanna Needell, University of California

**Abstract:** Recent advances in technology have led to a monumental increase in largescale data across many platforms. One mathematical model that has gained a lot of recent attention is the use of sparsity. Sparsity captures the idea that high dimensional signals often contain a very small amount of intrinsic information. Using this notion, one may design efficient low-dimensional representations of large-scale data as well as robust reconstruction methods for those representations. Binary, or one-bit, representations of data for example, arise naturally in many applications, and are appealing in both hardware implementations and algorithm design. In this talk, we provide a brief background to sparsity and 1-bit measurements, and present new results on the problem of data classification with low computation and resource costs. We illustrate the utility of the proposed approach on recently acquired data about Lyme disease.

# A New Approach to Inverse Scattering for Anisotropic Media

### Fioralba Calkoni, Rutgers University

### Abstract:

In the past thirty years the field of inverse scattering theory has become a major theme of applied mathematics with applications to such diverse areas as medical imaging, geophysical exploration and nondestructive testing. The growth of this field has been characterized by the realization that the inverse scattering problem is both nonlinear and ill-posed, thus presenting particular problems in the development of efficient inversion algorithms. Although linearized models continue to play an important role in many applications, the increased need to focus on problems in which multiple scattering effects can no longer be ignored has led to the nonlinearity of the inverse scattering problem playing a central role. In addition, the possibility of collecting large amounts of data over limited regions of space has led to the situation where the ill-posed nature of the inverse scattering problem becomes a problem of central importance. Initial efforts to deal with the nonlinear and ill-posed nature of the inverse scattering problem focused on the use of nonlinear optimization methods. Although efficient in many situations, their use suffers from the need for strong a priori information in order to implement such an approach. In addition, recent advances in material science and nanostructure fabrications have introduced new exotic materials for which full reconstruction of the constitutive parameters from scattering data is challenging or even impossible. In order to circumvent these difficulties, a recent trend in inverse scattering theory has focused on the development of a new approach, in which the amount of a priori information needed is drastically reduced but at the expense of obtaining only limited information of the scatterers. In this talk we present an overview of the aforementioned new ideas in the context of solving the inverse scattering problem for anisotropic inhomogeneous media. Our approach exploits properties of the linear scattering operator to decode non-linear information about the scattering medium, yielding mathematically justified and computationally simple reconstruction algorithms. We first show that the support of the scattering media can be rigorously characterized from the range of the scattering operator. The mathematical study of this operator is based on the analysis of a non-selfadjoint eigenvalue problem known as the transmission eigenvalue problem. Transmission eigenvalues relate to interrogating frequencies for which there is an incident field that does not scatter. We show that the transmission eigenvalues can be determined from the scattering data and provide information on the constitutive properties of the scattering media. Numerical examples will be presented to confirm the viability of our reconstruction algorithms.

### Claims Problems, a Progress Report

### William Thomson, University of Rochester

**Abstract:** When a firm goes bankrupt, how should its liquidation value be divided among its creditors? More generally, when a group of people have claims on a resource but there isn't enough of it to fully honor all of these claims, what should be done? The literature on the "adjudication of conflicting claims," which builds upon fascinating examples from antiquity and medieval times, has experienced a considerable development in the last few years. I will provide a short introduction to it and give a progress report on the recent research on the subject. The approach I will follow is mainly axiomatic. It starts with the formulation of elementary properties of allocation rules and seeks to understand the implications of these properties, when imposed in various combinations.

### Molecular-scale modeling and simulation of materials

### Eric Cancès, Ecole des Ponts ParisTech

**Abstract:** Molecular-scale modeling and simulation is one of the most dynamics area of scientific computing. It has a very broad field of applications, ranging from chemistry and drug design to solid-state physics, materials science and nanotechnology.

It is also a inexhaustible source of exciting mathematical and numerical problems of various nature: linear and nonlinear partial differential equations, optimization and control, stochastic processes and Monte Carlo methods, spectral theory, group theory, non-commutative algebra and geometry, statistical methods and machine learning...

In this talk, I will give an overview of some mathematical models and numerical methods used to predict macroscopic properties of a material from its atomic structure. I will first present the case of perfect crystals, where e.g. band structure diagrams constructed from Bloch-Floquet theory allow us to understand the difference in behavior between conductors, semiconductors, and insulators, as well as some of the properties of emerging topological materials. I will then discuss recent advances in the challenging field of modeling and simulating disordered systems such as crystals with defects, doped semiconductors, glasses, quasicrystals, or multilayer 2D materials.

### Random ordinary differential equations and their numerical approximation

### Peter Kloeden, University of Tuebingen

**Abstract:** Random ordinary differential equations (RODEs) are pathwise ordinary differential equations that contain a stochastic process in their vector field functions. They have been used for many years in a wide range of applications, but have been very much overshadowed by stochastic ordinary differential equations (SODEs). The stochastic process could be a fractional Brownian motion, but when it is a diffusion process there is a close connection between RODEs and SODEs through the Doss-Sussmann transformation and its generalisations, which relate a RODE and an SODE with the same (transformed) solutions. RODEs play an important role in the theory of random dynamical systems and random attractors. They are also useful in biology.

Classical numerical schemes such as Runge-Kutta schemes can be used for RODEs but do not achieve their usual high order since the vector field does not inherit enough smoothness in time from the driving process. It will be shown how, nevertheless, Taylor expansions of the solutions of RODES can be obtained when the stochastic process has Hölder continuous sample paths and then used to derive pathwise convergent numerical schemes of arbitrarily high order. RODEs with Itô noise will also be considered as well as RODEs with affine structure and Poisson noise. Applications to biology in will be given.

Xiaoying Han and P. E. Kloeden, Random Ordinary Differential Equations and their Numerical Solution, Springer Nature Singapore, 2017.

### Real Options and Differential Games in Commodity Finance

### Matt Davison, Western University

**Abstract:** Process Industries such as Mining, Energy, and Commodity Processing are the historical foundation of the Canadian economy. These industries typically utilize long-lived, expensive and large pieces of infrastructure. The profitability of projects in these industries depends on prices set on world commodity markets, but project operators often have considerable optionality in deciding when to open, close, run, or idle facilities. The question is, how to optimally utilize this operational flexibility and how to value projects in the face of it. The resulting problems are mathematically quite similar to American Options problems from traditional Quantitative Finance, but often involve more complicated modelling around cost structures to idle a run plant or to restart an idled plant. In addition, particularly in rather local energy markets, the impact of idling a plant can significantly impact market prices, leading to interesting multi-player dynamic, or differential, games.

This talk will focus on the mathematical, economic, and financial insights my co-workers and I have found over nearly 20 years of working in this area, in areas including hydroelectric power, to natural gas storage, to corn ethanol production, to shipping of oil and liquefied natural gas.

### Quality of Electronic Health Databases for Real-World Evidence Studies

### Lisa Lix, University of Manitoba

Abstract: Canada is a world leader in the creation, linkage, and use of population-based electronic health databases to support healthcare decision making. However, there are challenges in using electronic health databases to improve our understanding of health. These databases were developed to monitor patient care and manage the healthcare system; they were not intended to be used for research. Accordingly, the information contained in electronic health databases is often of poor quality for real-world studies; it lacks standardization and documentation, and frequently contains inaccurate and inconsistent information. In this talk, methods to combine electronic health data from multiple sources or time periods to improve the accuracy of health measures will be discussed, including imputation models, latent variable models, and various approaches to data validation. Activities to automate data quality evaluations will be described. Examples from provincial and national chronic disease research and surveillance projects will be used to illustrate the challenges and opportunities.

### Tools for Mapping and Controlling the Brain

### Edward Boyden, Massachusetts Institute of Technology

Abstract: To enable the understanding and repair of complex biological systems such as the brain, we are creating novel optical tools that enable molecular-resolution maps of large scale systems, as well as technologies for observing and controlling high-speed physiological dynamics in such systems. These tools may enable datasets for precision modeling and control of the brain, at a computational level. First, we have developed a method for imaging large 3-D specimens with nanoscale precision, by embedding them in a swellable polymer, homogenizing their mechanical properties, and exposing them to water – which causes them to expand isotropically manyfold. This method, which we call expansion microscopy (ExM), enables scalable, inexpensive diffraction-limited microscopes to do large-volume nanoscopy, in a multiplexed fashion - important, for example, for brain mapping. Second, we have developed a set of geneticallyencoded reagents, known as optogenetic tools, that when expressed in specific neurons, enable their electrical activities to be precisely driven or silenced in response to millisecond timescale pulses of light. We have also begun to develop noninvasive ways to electrically stimulate deep targets in the human brain. Finally, we are developing novel reagents, such as fluorescent voltage indicators, and systems, such as novel microscope architectures, to enable the imaging of fast physiological processes in 3-D with millisecond precision. In this way we aim to enable the systematic mapping, control, and dynamical observation of complex biological systems like the brain, with the ultimate goal of enabling detailed computational models of brain circuits and computational principles of neural control.

# Semi-Plenary Lectures

### New Results on the Erdös-Selfridge Function g(k)

### Jon Sorenson, Butler University

**Abstract:** Let q(k) be the smallest integer larger than k+1 such that the binomial coefficient C(g(k), k) has no prime divisors  $\leq k$ . So for example, we have g(2) = 5, since C(5, 2) = 15, and 15's smallest prime divisor is 3. Also we have g(3) = g(4) = 7, since C(7,3) = C(7,4) = 35, and 35's smallest prime divisor is 5. The problem of estimating q(k) has interested number theorists since Paul Erdös introduced the problem back in 1969. For example, Richard Guy mentions the problem in his well-known book Unsolved Problems in Number Theory. Ecklund, Erdös, and Selfridge published the first paper on this problem back in 1974, where they proved upper and lower bounds on g(k), stated several conjectures on its behavior, and tabulated g(k) for k up to 40, plus g(42), g(46), and g(52). The best current upper bound,  $g(k) < \exp[k(1+o(1))]$ , is from this same 1974 paper. The best current lower bound,  $g(k) > \exp[c(\log k)^2]$  for an absolute constant c > 0, is due to Konyagin (1999). Others who published lower bounds for g(k), all in the 1990s, include Lacampagne, Granville, and Ramaré. Scheidler and Williams (1992) described how to use Kummer's theorem to construct a sieving algorithm to compute g(k), and computed g(k) for all  $k \leq 140$ . Finally, Lukes, Scheidler, and Williams (1997) improved their sieve and computed g(k) for all  $k \leq 200$ . A complete table of known values of g(k) is available from the Online Encyclopedia of Integer Sequences (A003458) at https://oeis.org/A003458/.

In this talk, we present some new results and work-in-progress on g(k). We have a new sieve algorithm to compute g(k), based on a wheel datastructure that was used previously to find pseudosquares, pseudoprimes, and primes in patterns. This algorithm runs in time sublinear in g(k), and we used it to find g(k) for all k up to 272 so far. In particular we have  $g(272) = 57\,61284\,34192\,78614\,55093\,37498.$ 

Let M = M(k) be the product of the primes  $p \leq k$ , raised to the power  $\lfloor \log pk \rfloor + 1$ , and let R = R(k) be the number of acceptable residues modulo M under Kummer's theorem. Our unproven Uniform Distribution Heuristic states that the smallest acceptable residue modulo Mis roughly M/R, which implies that  $\log g(k) = \log(M/R) + O(\log k)$  with high "probability." We then show unconditionally that  $\log(M/R)$  is roughly  $k/\log k$ , or more specifically, that the ratio of  $\log(M/R)$  over  $k/\log k$  is, in the limit, at least  $(1-\log 2)/2$ , and at most 2. The data from our computations supports this so far, and in fact, our data implies that  $g(k) \approx \exp[1.19k/\log k]$ .

This is joint work with Brianna Sorenson (undergraduate student) and Jonathan Webster, both of Butler University.

### The "Waterloo Fractal Analysis and Coding Project": Generalized fractal transforms, contraction maps and associated inverse problems

### Edward R. Vrscay, University of Waterloo

Abstract: Originally inspired by the work of B. Mandelbrot, who showed that classic "fractal sets" could be viewed as unions of contracted copies of themselves, as well as the idea of generating fractal sets using systems of contraction mappings, our "Waterloo Fractal Analysis and Coding Project" has, over the past 30 years, been interested in "generalized fractal transforms" (GFTs) over various spaces. A GFT, T, defined on a complete metric space (X, d) acts on an element (X, d) in the following "fractal-like" way: It first makes N modified copies of x (e.g., spatially-contracted, range-transformed and translated), then combines these "fractal components,"  $x_i$ , in a manner appropriate to the space X, to produce a new element y = Tx.

Under certain conditions, the operator T is contractive on X which, from Banach's Fixed Point Theorem, implies the existence of a unique fixed point p = Tp. From the action of T, p is "self-similar" in the sense that it is an appropriate combination of modified copies of itself. In the 1990's, fractal image coding naturally led to the formulation of GFTs on various function spaces. This naturally leads to associated GFTs on Fourier and wavelet transforms. More recently, we have looked at GFTs on multifunctions, as well as function- and measure-valued mappings, both of which have applications in image processing, as will be briefly discussed.

We also have been concerned with the following inverse problems associated with contraction mappings: Let Con(X) be a class of contraction maps on a complete metric space (X, d) (e.g. GFT's). Then given an  $x \in X$ , can one find a map  $T \in Con(X)$  with fixed point p sufficiently close to x? This is the essence of fractal image coding and compression: We approximate an image x with p and then store the the parameters that define T – the so-called "fractal code" of x. The approximation p can then be generated by iteration. Fractal image coding seems to work, in other words, images do possess a kind of self-similarity, which will be discussed briefly.

However, finding a map T by trying to make the approximation error d(x, p) small is generally intractable. Thanks to a very simple consequence of Banach's Theorem – known in the fractal coding literature as the "Collage Theorem" – one looks for a contractive map T that minimizes the so-called "collage distance" d(x, Tx).

Such collage-based methods are also applicable in "nonfractal" situations, for example, inverse problems in ODEs, PDEs and inclusions, In fact, it didn't take long for the "nonfractal" applications to outnumber the "fractal" ones!

# Field control in exterior regions through surface sources

# Daniel Onofrei, University of Houston

**Abstract:** In this talk we will present our results concerning the problem of exterior field control through surface currents with applications to pattern synthesis, scattering cancellation and design of essentially non-radiating sources. We will first offer a brief review of our existent results concerning the control of scalar fields and then discuss how these controls can be used for Maxwell fields. We will then present current results for the control of the electromagnetic fields together with numerical simulations for various applied scenarios.

# AMMCS Prize-Winning Lecture

# Kolmogorov–Wiener Prize for Young Researchers Some Mathematical Advances in Computational Techniques for Liquid Crystal Modeling

## David Emerson, Street Contxt & Tufts University

Abstract: As materials possessing mesophases with characteristics of both liquids and organized solids, liquid crystals exhibit an array of interesting physical properties, including dielectric and flexoelectric coupling, inspiring a wide range of applications. In addition to prevalent use in modern display technologies, liquid crystals are applied, for example, to nanoparticle organization, the manufacture of nanoporous solids, and the design of effective actuators, such as light driven motors and artificial muscles. Accurate and efficient numerical simulation of liquid crystal behavior is used to optimize device design, analyze experiments, and suggest the presence of new physical phenomena. Mathematical models of liquid crystals present a number of interesting challenges for the design of theoretically supported computational techniques. Such challenges include highly nonlinear systems, point-wise unit-length constraints, strong coupling with electric and hydrodynamic effects, and stable configurations incorporating discontinuities, among others. In this talk, we focus on the Frank-Oseen model of liquid crystals, introducing the elastic model for equilibrium configurations, its extension incorporating electric fields, and briefly discuss the addition of hydrodynamic effects. We consider the construction of theoretically supported approaches for such systems and examine a number of methods aimed at addressing different aspects of efficient simulation ranging from well-posed finite-element discretizations to reliable a posteriori error estimators. These methods expand the existing set of computational tools available for effective simulation of liquid crystal behavior. Finally, we highlight some of the interesting open questions and ongoing work in this area. This is joint work with a number of collaborators including James Adler and Tim Atherton (Tufts), Scott MacLachlan (Memorial), Patrick Farrell (Oxford), and Tom Manteuffel (Colorado Boulder).

# Session Presentations

### **Covering Large Complex Networks by Cliques - A Sparse Matrix Approach**

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Identification of and computation with dense or otherwise highly connected subgraphs are two of the kernel operations arising in areas as diverse as sparse matrix determination and complex network analysis [1, 5]. In social network analysis, identification of special interest groups or characterization of information propagation in the network denote two examples of frequently performed operations. Finding efficient representations of network data and designing new algorithms that scale well with the problem instance size are both central to meeting challenges in the analysis of massive data sets using graph theoretic abstractions.

Let G = (V, E) be an undirected connected graph with |V| = n vertices and |E| = m edges. A clique is a subset of vertices such that every pair of distinct vertices are connected by an edge in the induced subgraph. We are concerned with finding a decomposition, a clique cover, of graph G into complete subgraphs such that each edge is included in at least one of the subgraphs. The problem of finding a clique cover with minimum number of cliques (and variants of the same) is known to be NP-hard (see [2]). In this work we propose a compact representation of network data based on sparse matrix data structures [3] and provide efficient implementation of new and existing heuristics for clique cover. Our proposed solution is based on the simple but important observation that for a sparse matrix  $A \in \mathbb{R}^{m \times n}$ , the column intersection graph of A is isomorphic to the adjacency graph of  $A^{\top}A$ , and that the row intersection graph of A is isomorphic to the adjacency graph of  $AA^{\top}$  [4]. Consequently, the subset of columns corresponding to nonzero entries in row i induces a clique in the adjacency graph of  $A^{\top}A$ , and the subset of rows corresponding to nonzero entries in column j induces a clique in the adjacency graph of  $AA^{\top}$ . Note that, matrices  $A^{\top}A$  and  $AA^{\top}$  are most likely dense even if matrix A is sparse. Thus, given a graph G = (V, E), the objective is to find a suitable family of vertex-induced complete subgraphs  $\{G_1 = (V_1, E_1), \dots, G_k = (V_k, E_k)\}$  such that V = $\bigcup_{i=1}^{k} V_i$  and  $E = \bigcup_{i=1}^{k} E_i$  and that the number of subgraphs k is minimized. Sparse matrix representation of network data allows us to express graph operations in terms of sparse linear algebra primitives, enabling improved locality of reference for data access in modern multi-level hierarchical memory architecture and exploiting parallelism in many-core computing systems [1, 4]. We provide details of a reference implementation and results from extensive numerical testing.

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# Modelling the daily risk of Ebola virus in the presence and absence of a potential vaccine

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Ebola virus — one of the deadliest viral diseases, with a mortality rate around 90% — damages the immune system and organs, with symptoms including episodic fever, chills, malaise and myalgia [1, 2]. The Recombinant Vesicular Stomatitis Virus-based candidate vaccine (rVSV-ZEBOV) has demonstrated clinical efficacy against Ebola in ring-vaccination clinical trials [3]. In order to evaluate the potential effect of this candidate vaccine, we developed risk equations for the per-day risk of Ebola infection both currently and after vaccination. The risk equations account for the basic transmission probability of Ebola and the lowered risk due to various protection options: vaccination, hazmat suits, reduced contact with the infected living and dead bodies. Parameter space was sampled using Latin Hypercube Sampling, a statistical method for generating a near-random sample of parameter values [4]. We found that at a high transmission rate of Ebola (i.e., if the transmission rate is greater than 90%), a large fraction of the population must be vaccinated (> 80%) to achieve a 50% decrease in the daily risk of infection. If a vaccine is introduced, it must have at least 50% efficacy, and almost everyone in the affected areas must receive it to effectively control outbreaks of Ebola. These results indicate that a low-efficacy Ebola vaccine runs the risk of having vaccinated people be overconfident in a weak vaccine and hence the possibility that the vaccine could make the situation worse, unless the population can be sufficiently educated about the necessity for high vaccine uptake.

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# An Optimal Control Strategy for a Malaria Model

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Malaria is a major vector-borne disease that has been generating a serious health burden and devastating the economy of Sub-Saharan Africa, South-East Asia and the Eastern Mediterranean. In this paper, a mathematical model for control of malaria in low and high-risk human population groups, incorporating four control variables representing insecticide treated nets, treatment, indoor residual spraying and intermittent preventive treatment of malaria in high-risk human population; seasonally forced mosquito population and transmission parameters, is formulated. The necessary conditions for the optimality of the model are derived using the Pontryagin's Maximum Principle. The optimal control model is numerically explored using Runge-Kutta method of order four. Experimental results show that the model is able to indicate the best control strategy, given the estimated costs of implementation of the varying control measures.

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# Secure and efficient multiparty quantum secret sharing with five-qubit brown states

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Cryptography is one of the most important branches of information technology, which is becoming increasingly important day by day to secure sensitive data. Secret sharing, which was invented by Shamir in 1979 [1], is an efficient and reliable technique of cryptography. In the classical secret sharing scheme, the boss Alice wants to distribute a secret among N agents in such a way that only by combining their shares can the N agents recover the secret massage. Also, the secret sharing scheme enables the honest agent to prevent the dishonest one from occurring any damage. Secret sharing has many useful applications which can be applied in networkbased scenarios, such as secure money transfer, remote voting, auctioning, and secure multiparty computation.

Unfortunately, with the development of quantum computing algorithms [2] which will be applied by a powerful quantum computer [3], most cryptographic protocols that rely on mathematical complexity will not be longer safe. To solve the problem of traditional secret sharing schemes, a quantum secret sharing (QuSS) scheme as an interesting aspect of quantum cryptography [4] was suggested by Hillary et al. [5] in 1999. QuSS can be used to share quantum states or classical information securely. In the QuSS, the quantum operation is utilized to distribute secret information among legitimate participants.

In this work, we present a secure and efficient multi-party QuSS scheme with five-qubit brown states. The boss encodes his/her secret by applying three single-qubit local unitary operations on only three qubits of each five-qubit brown state. Finally, the legitimate participants (agents) measure the brown states and decode the measurement results to recover the shared secret key effectively. The security analysis of the proposed QuSS protocol proves that it can resist against both inside and outside attacks. Compared with existing QuSS protocols, the proposed protocol also has a higher information efficiency and more feasible since it only requires single-qubit measurements.

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## An Efficient Model for Integrating Public Participation in the Solid Waste Collection Vehicle Routing Problem

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One of the major challenges facing municipal waste management teams relates to the development of an efficient vehicle routing across the customers' locations such that all customers' requests are satisfied daily. However, the success of daily collection of solid wastes has always been affected by a few events such as: limited available vehicles, traffic delays, vehicle breakdowns, scheduled maintenance and uncertainties associated with drivers' availability. A possible approach for mitigating the occurrence of any of these events is to involve public participation in the routing process. In this paper, a new mathematical model for integrating the participation of standby drivers into the routing procedures is proposed. The standby drivers operate their own vehicles which are identical to the fleet of homogeneous vehicles hosted at a fixed depot. A standby driver is compensated depending on the number of customers visited and the total distance covered. Using the collection of solid waste such that each customer is visited exactly once, and all the requests are satisfied daily. A simple Lagrangian heuristic is developed to implement the model using standard related benchmark problem instances and randomly generated data-sets for a hypothetical case study. Preliminary results show that the model is efficient, while the heuristic algorithm was able to find feasible solutions in very good times.

# **Estimation of Parameters of a Constrained Predator Prey Dynamical Model with Incomplete Data**

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Substantial frameworks for estimation of parameters of a predator prey dynamical model have been developed in the past. in this research, method for estimating parameters of a constrained dynamical model with incomplete data by assuming information about predator is known and prey is unknown was investigated. In addition, method of undetermined Langrangian multiplier was applied to estimate the unknown parameters. The method for estimating the parameters was based on the construction of a quadratic goal function from a set of ordinary deferential equations (ODEs) and its minimization. A non-homogeneous system was generated using ordinary least square method which was applied to the goal function in order to recover the parameters. The derivation of the parameters process was one of the inverse problems investigated and the estimated parameters gave some satisfactory results. It is also discovered that in real life situations there are some dynamical systems whereby its not possible to solve for a variable with respect to the other and this need to be investigated in the future.

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#### A first-order system finite-element method for boundary layer problems

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We are interested in finite-element solutions of singularly perturbed problems, whose solutions feature boundary layers. There has long been concern that finite-element analyses are not appropriate for such problems, since it is often the case that the natural energy norms associated with standard Galerkin methods are not strong enough to represent the layers present in the solution. Lin and Stynes (SINUM, 2012) were among the first to fully diagnose the key issue that, for a reaction- diffusion problem, the energy norm is not correctly "balanced". They also proposed a remedy, in the form of a mixed finite element method, for which the associated norm is balanced.

There have been various other attempts to either prove the convergence of solutions obtained with standard methods, but in non-induced norms, or to devise new schemes; see, e.g., Roos (Proc. BAIL 2016) for an overview. Our interest is in the latter approach and, in particular, in the method proposed by Adler et al. (IMA J. Numer. Anal., 2016). This has advantages over the Lin and Stynes approach, including that the associated finite-element space is simplified, and that one can apply fast solvers.

In this talk, we will examine how that framework can be enhanced so that it may provide further advantages, including being extendable to other other singularly perturbed problems, and allowing natural adaptive refinement.

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## The journey of a single polymer chain to the entrance of a nanopore

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Dynamics of polymer molecules while going through a nanopore has been a hot topic for over two decades due to its applications in studying biomolecules, especially DNA sequencing and electrophoresis. For a molecule to successfully get to the other side of a porous media, it must first find the entrance. In most of the previous studies, researchers showed interest in characterizing the motion of the macromolecule when it has already found the pore. However, we think there is more to this process. We observed that the dynamical behaviour of a polymer chain under non-uniform pressure-driven flow is different from usual Langevin dynamics and the flow impacts the conformation of the molecule in a way that helps it to find the channel entrance. In our paper, we investigate conformational characteristics of a general polymer molecule and the flow field surrounding it, using hybrid molecular dynamics-lattice Boltzmann simulation, to find the clear relation between the flow field and the polymer molecule conformations travelling under that flow.

## Model of a Cortical Circuit Associated with Childhood Absence Epilepsy

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Childhood absence epilepsy (CAE) is a common idiopathic pediatric epilepsy disorder characterized by brief episodes of impaired consciousness. Patients typically demonstrate bursts of synchronous 2.5-4 Hz spike-and-wave activity on the electroencephalogram (EEG), a tool commonly used to classify epilepsy type [1]. The thalamocortical circuit, consisting of the cortex and thalamus, is considered to play an important role in the pathophysiology of AE, exhibiting the ability to generate oscillations of different frequencies and a range of synchrony [2]. The cortex, in particular, is integral in the development of spike-and-wave discharges. Connectivity with the cortex ensures that with sufficient corticothalamic feedback, the circuit behaviour can switch from high-frequency mode of oscillations to a slower and hypersynchronized mode, demonstrating spike-and-wave EEG patterns [3]. Genetic rodent models of AE provide evidence of a cortical focus initiating rhythmic discharges, which then recruits the thalamus to keep the discharges sustained [4]. To understand sustainment of oscillations and hypersynchrony in the cortex associated with AE, we use a small network of cortical pyramidal neurons and an interneuron each described by a single-compartment Hodgkin-Huxley style model. By taking into account the layered nature of the cortex, and by varying the external input current and synapse strengths, we investigate conditions required for the network to maintain synchrony. As well, we explore the role of genetic defects at the single-neuron level, in the development of an epileptogenic network.

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# **Tunable Directional Plasmon Excitation and Transition Radiation in Phosphorene by a Swift Electron**

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The emergence of two-dimensional (2D) crystals that took place in recent years has been regarded as a platform that may impact future photonic science and electronic technologies [1]. Initially, graphene has attracted enormous amount of interest in plasmonic and optoelectronic research owing to its low-energy electronic band structure being akin to the massless Dirac fermions, its high carrier mobility, and the dynamic tunability of its doping density. The invention of phosphorene as a monolayer of black phosphorus, on the other hand, which shows semiconducting properties with a thickness dependent (i.e., highly tunable) band gap, a strong in-plane anisotropy (particularly the anisotropy of electric conductance), and high carrier mobility, offers improvements for many technological concerns regarding 2D materials [2].

As regards the plasmonic properties of 2D materials, Electron energy loss spectroscopy has become one of the most widely used analytical techniques that measures the dynamic polarization of a 2D material by a fast electron beam in a broad range of frequencies [3, 4]. Considering the isotropy of graphene polarization by a normally incident electron beam, graphene-based radiative and plasmonic applications are expected to offer relatively isotropic radiation patterns and surface plasmon modes in all spatial directions [5, 6, 7]. This intuitive argument calls for attention to study interactions of an external charged particle with a strongly anisotropic sheet, such as phosphorene, in the retarded regime. In particular, using an oblique incidence of the charged particle could reveal how the more exotic collective modes in anisotropic 2D materials may affect the energy loss spectra of the incident particle and the directional patterns of the emitted electromagnetic (EM) radiation from the target [8].

In this work, we assume an obliquely incident external electron traversing phosphorene, enabling us to explore the effects of the anisotropy of the sheet on the efficiency of the plasmon excitations and the angular anisotropy of the emitted transition radiation spectra as a function of the incident particle direction relative to the principal directions of the sheet. Accordingly, in addition to the incident particle energy, its angle of incidence is established as an important quantity that may be considered as a significant tuning parameter for the EM response of the anisotropic sheet.

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#### On the Lang-Trotter Conjecture for two elliptic curves

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Following Lang and Trotter [4] we describe a probabilistic model that predicts the distribution of primes p with given Frobenius traces at p for two fixed elliptic curves over  $\mathbb{Q}$ . In addition, we propose explicit Euler product representations for the constant in the predicted asymptotic formula and describe in detail the universal component of this constant. A new feature is that in some cases the  $\ell$ -adic limits determining the  $\ell$ -factors of the universal constant, unlike the Lang-Trotter conjecture for a single elliptic curve, do not stabilize. We also prove the conjecture on average over a family of elliptic curves, which extends the main results of [3] and [1], following the work of David, Koukoulopoulos, and Smith [2].

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## **Computational Study of Secondary Neutrons Produced by Protontherapy**

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In radiation therapy, some of the uncertainties can be addressed by physics, such as uncertainties due to dose calculation. Dose calculations are routinely performed using analytical algorithms that are fast enough to allow treatment optimization in minutes. While these techniques are typically sufficiently accurate in the photon world, they have significant shortcomings in proton therapy[1]. The steeper dose gradients present in particle fields expose the approximations in analytical algorithms, in particular with respect to scattering of protons at interfaces such as bone and soft tissue. While too slow to be used in the clinic in the past, dose calculations based on particle-track simulations ('Monte Carlo') have recently achieved efficiencies that make them suitable for use in treatment planning[2]. Monte Carlo codes offer superior dose calculations to analytical algorithms and are considered the gold standard[3]–[6].

In protontherapy still there are some important physics challenges like range, dose uncertainties, and secondary neutrons produced by proton and carbon-ion beams in materials of beam-line elements, collimators, range modulators and also in the treatment volume. Such neutrons propagate further in surrounding tissues, air and shielding of the treatment room and can deposit energy very far from their production points. These neutrons have a higher Relative Biological Effectiveness than photons. Therefore, side effects to the patient may occur. For instance, the secondary neutron is one of the factors that increase the integral dose, which can lead to the patient's secondary cancer.

This study focus on the characteristics of the secondary neutrons dose, which produced as an undesirable result during the protontherapy in the treatment area, and investigate the feasibility to utilize the thermal neutron for Boron Neutron Capture Therapy (BNCT). The study has been done by using Monte Carlo N-Particle Code (MCNP) to model and estimate/ calculate the proton dose and the total amount of secondary neutrons and their energy ranges.

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### Phase Models with Large Time Delayed Coupling

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In this talk, we consider a weakly connected system of two identical coupled oscillators with time delayed coupling

$$\frac{d\mathbf{X}_{1}}{dt} = \mathbf{F}(\mathbf{X}_{1}(t)) + \varepsilon \mathbf{G}(\mathbf{X}_{1}(t), \mathbf{X}_{2}(t-\tau)),$$

$$\frac{d\mathbf{X}_{2}}{dt} = \mathbf{F}(\mathbf{X}_{2}(t)) + \varepsilon \mathbf{G}(\mathbf{X}_{2}(t), \mathbf{X}_{1}(t-\tau)),$$
(1)

such that when there is no coupling in the network ( $\varepsilon = 0$ ) each oscillator has a unique exponentially asymptotically stable limit cycle with period *T* and corresponding frequency  $\Omega$ . Let  $\eta := \varepsilon \Omega \tau = \mathcal{O}(1)$  for sufficiently small  $\varepsilon$ . Then, by applying weakly coupled oscillator theory with delayed interactions as in [1], we reduce (1) into the phase deviation model

$$\frac{d\varphi_1}{dt} = \frac{1}{\Omega} H(\varphi_2(t-\eta) - \varphi_1 - \Omega\tau), 
\frac{d\varphi_2}{dt} = \frac{1}{\Omega} H(\varphi_1(t-\eta) - \varphi_2 - \Omega\tau),$$
(2)

where the phase interaction function *H* is explicitly defined in terms of *G* and the uncoupled limit cycle in (1). In (2), we study the existence and (local) stability of solutions of the form  $\varphi_1 = \omega t$  and  $\varphi_2 = \omega t + \psi$  where  $\omega$  is the phase deviation of the oscillator and  $\psi$  is the natural phase difference. As a numerical example, we consider

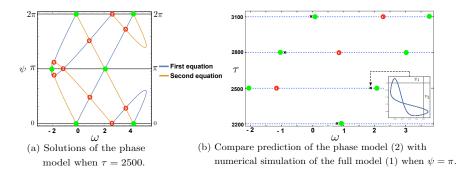


Figure 1: The circle  $\bullet/\circ$  represents stable/unstable solutions in the phase model corresponding to Morris-Lecar model and  $\times$  represents the calculated  $\omega$  in Morris-Lecar model.

the Morris-Lecar model with two sets of parameter values from [2]. We discuss the stability and bifurcations of solutions in the phase model, and compare prediction of the phase model (2) with numerical simulations of the full model (1), see Figure 1. Moreover, we consider small time delay, in the sense that,  $\Omega \tau = \mathcal{O}(1)$  with respect to  $\varepsilon$ , and compare the results with [2] where the authors studied this case.

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#### SIR Model with Time-Varying Contact Rate

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The contact rate is defined as the average number of contacts adequate for disease transmission by an individual per unit time; and it is usually assumed to be constant in time [1]. However, in reality, the contact rate is not always constant throughout the year due to different factors such as population behaviour, environmental factors and many others [2]; therefore it is more realistic to be considered as a function of time. For example, F. Brauer in [3] assumed that the contact rate decreases exponentially in time because of individual behavioral changes in response to a disease outbreak.

In this work, we assume that the number of contacts decreases in time till certain level, and then remains constant. This assumption is more realistic than assuming a contact rate that decreases exponentially. For this purpose, we consider the contact rate  $\beta(t)$  to obey the following differential equation:

$$\beta' = -c \left(\beta(t) - \beta_2\right) \left(1 - \frac{\beta(t) - \beta_2}{\delta\beta}\right) \tag{1}$$

Here  $\beta_2 < \beta(t) < \beta_1$ ,  $\delta\beta = \beta_1 - \beta_2$ , and -c < 0 represents the decay rate of the contact rate. Our aim is to study SIR model with time-varying contact rate described by differential equation (1). The existence and local stability of the equilibria of the model are analyzed. Results on global stability of disease-free equilibrium and transcritical bifurcation are proved. Finally, numerical simulations are presented to illustrate the theoretical results and to demonstrate the effect of the model parameters related to the behavior of the contact rate on the model dynamics.

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# A Mathematical Model for Equation of State Effects Relevant to Nano-Cellular Polymeric Foams

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Polymeric foams are widely used in industry to enhance material strength, reduce product weight and manufacturing cost. Accurate modelling of equation of state effects is critical to predicting conditions favourable to achieving nanometer cell sizes in the foams. A complete equation of state should be able to predict density as well as the glass transition behaviour of polymeric foams since glass transitions play a significant role in determining polymeric foam cell sizes and are central to a phenomenon called retrograde vitrification that allows polymers to plasticize at milder conditions. In retrograde vitrification a polymeric foam state changes from glassy to liquid due to *decrease* in temperature of the polymeric foam provided that a high soluble foaming gas is used.

To describe these behaviours, we have proposed a mathematical model that is based on an off-lattice treatment of the Sanchez-Lacombe equation of state. This model associates two energy levels with the finite flexibility of polymer chains. Consequently, this model successfully captures pressure-volume-temperature behaviour and a sudden increase in isobaric heat capacity of polymer systems that is observed experimentally. However, the theoretical heat capacity is in qualitative agreement with experimental data. Efforts to achieve quantitative matching are underway.

## **Epidemic Dynamics of Vector-Transmitted Diseases: Analysis of the Vector-to-Host and Host-to-Vector Forces of Infection**

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We study a class of models for vector-transmitted diseases by analyzing the forces of infection formulated as a coupled system of renewal equations. We derive the basic reproduction number and a final size relation for a closed vector and host population. We extend the model to the case where both vector and host populations have demographic dynamics and derive the positive equilibrium and its local stability.

# Latin Hypercube Sampling and the Sensitivity Analysis of Hepatitis B-viral Models

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Due to uncertainties in experimental data used to estimate parameter values, the accuracy of results from both mathematical and computer models of biological systems is often an intricate matter. Sensitivity analysis (SA) may help in identifying strongly influential model parameters, targeting experimental focus on these key parameters and thus optimizing the model's structure. In particular, infectious disease modeling benefits from the adoption of global SA techniques capable of providing considerable insight beyond traditional local sensitivity analysis techniques. In this article, a Latin hypercube sampling (LHS)- based sensitivity study is conducted for two models: (a) single hepatocyte HVB model [2] and (b) multi-scale spatial HVB model [1]. Both models describe the viral dynamics and clearance of hepatitis-B in the liver. Virons are converted to the covalently-closed circular DNA (cccDNA) and then to relaxed' viral DNA (rcDNA), double- strand' viral DNA (dsDNA) and protein p36, the most important component for viral replication and aggravation of infections. The LHS method provides information, especially over time, on the quantitative relationship between parameters and model output. For both models, the sensitivity analysis suggests that the transportation rate of protein p36 is the most influential on cccDNA replication, resulting in severe liver infection.

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# Sensitivity of shale gas transport model to changes in the pressure dependent parameters

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A new nonlinear transport model for the flow of gas in tight porous media, such as shale rock formations, has been proposed by the authors [1, 2], see also [3]; it was shown to predict shale rock properties with greater accuracy than previous models. A key feature in this model is that all model parameters are kept and fully pressure dependent throughout the simulations. Here, we investigate the sensitivity of the model to small changes in parameters as applied to pressure-pulse tests in shale rock samples for different pressure inflow,  $P_{in}$ , conditions. For high  $P_{in}$ the results become critically sensitive to some of the parameters, but not to others, Fig 1. A simplified modeling strategy is proposed in which some of the non-critical parameters are kept constant, and the results obtained reasonably approximate the pressure dependent full model. We infer that for the best estimates of rock properties from pressure-pulse tests you need high Pin conditions; the model is not very sensitive to model parameters for low levels of inflow pressures  $P_{in}$ .

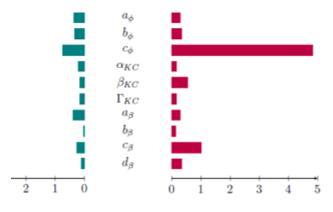


Figure 1: Sensitivity to different model parameters.

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#### Shortcuts to Adiabaticity in Driven Open Quantum Systems

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Shortcuts to adiabaticity (STA) allow one to control the evolution of a quantum system without the requirement of slow driving. The controlled speedup of quantum process is broadly recognized as a necessity for the advance of quantum technologies and STA have found a variety of applications, including phase-space preserving cooling, population transfer, and friction suppression in finite-time thermodynamics, to name some relevant examples.

Despite this remarkable progress, the use of STA has been predominantly restricted to tailor the dynamics of isolated driven systems. Any physical system is however embedded in a surrounding environment with which it can interact and exchange energy, particles, etc. In such setting, the dynamics of the system is no longer-described by a Hamiltonian and is associated with a master equation.

We introduce a general scheme to engineer STA in arbitrary open quantum systems. We consider the evolution of a quantum system described by a mixed state along a prescribed trajectory of interest. We then find the equation of motion that generates the desired dynamics. It is found that the latter can be recast in terms of the nonlinear evolution of a system in the presence of balanced gain and loss. Alternatively, the dynamics can be associated with a non-Markovian master equation with time-dependent Lindblad operators whose explicit form is determined by the prescribed trajectory. As an illustration we engineer superadiabatic cooling, heating and isothermal strokes for a two-level system.

#### **Domination of Stable Allocations as a Fairness Criterion**

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We study the school choice problem: the allocation of indivisible goods that are associated with priorities over the agents who may consume them. Stability has been the main normative consideration in the literature on such problems [1]. However, depending on the priority structure, stability may be incompatible with Pareto-efficiency. We offer an alternative criterion for fairness: rather than insist on an allocation being stable itself, it ought to be deemed fair if it Pareto-dominates a stable allocation. We call such allocations *stable-dominating* allocations.

When priorities are strict, there exists a unique agent-optimal stable allocation for every profile of preferences. Moreover, for such priorities, the set of stable allocations satisfies the "Rural Hospitals Theorem," which states that an agent is assigned to a school at one stable allocation if and only if she is assigned to school at *every* stable allocation [2]. Finally, when priorities are strict, the rule that selects the agent-optimal stable allocation is strategy-proof (that is, it provides incentives for every agent to truthfully report her preferences) [3]. Our first set of results establish that given a priority structure, whether it is strict or not, the following statements are equivalent:

- 1. There exists an agent-optimal stable allocation for every profile of preferences for said priority structure.
- 2. For said priority structure, A) there is a unique stable-dominating and strategy-proof rule and B) the Rural Hospitals Theorem holds.

Next, a structural result on the set of allocations help us to better understand the stable-dominating set. We show that if an allocation Pareto-dominates a non-wasteful allocation, then A) every agent is assigned to a school at the dominating allocation if and only if she is assigned to a school at the dominated allocation, B) every school is assigned to the same number of agents by both allocations, and C) if a school is not filled to capacity by the dominated allocation, then it is assigned to precisely the same agents by the dominating allocation. Using this result, we characterize the priority structures for which the stable-dominating set is equivalent to the stable set. The condition on priorities that guarantees this is slightly stronger than the acyclicity condition of [4].

Finally, we show consider the stronger incentive property of *group strategy-proofness*. This requires a rule to be immune to collusive misreporting of preferences by groups of agents. We show that a stable-dominating rule can be group strategy-proof only if it is actually stable.

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#### Reduction of queuing delay in internet traffic

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Congestion control is among the most fundamental problems in computer networking. With the networks becoming increasingly complex and saturated, efficient control of internet traffic congestion has become more important than ever. Transmission Control Protocol (TCP) is a set of procedures that facilitate reliable data transfer across a network. TCP is reliable in the sense that any segment of data that is lost or corrupted is retransmitted, and all packets of data arrive at the destination in the order that they are sent. Although TCP guarantees reliable data delivery, the physical and computational limitations of network hardware and software cause congestion resulting in wasted resources and transmission delays [1].

The development of a dynamic model of TCP has encouraged the application of control principles to Active Queue Management (AQM) schemes [3]. In particular, [2] has demonstrated that the inherent presence of the queuing delay in the traffic cannot be ignored and approached it as an optimal control problem of a statedependent delay system. In this paper we applied recently developed Model-free control (MFC) [4] strategy to reduce congestion. While traditional approaches rely on the accuracy of the TCP behavior model, MFC is robust against modeling errors. Simulation results show that our control algorithm can effectively reduce the queue length even in the presence of measurement noise. Mathematical analysis and numerical simulation results of our control algorithm will be presented. Moreover, the potential applicability as well as the limitations of model-free control methods in systems with inherent state-dependent and input-action delay will be discussed.

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#### Analysis of Methods for the Maxwell-Random Lorentz Model

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Electromagnetic wave propagation in complex dispersive media is governed by the time dependent Maxwell's equations coupled to equations that describe the evolution of the induced macroscopic polarization. In this work [1], we consider linear dispersive media described by a Lorentz model for electronic polarization which treats electrons in the material as damped harmonic oscillators. We relax the assumption that the material response will be well-represented by this Lorentz model using constant parameters by considering "polydispersive" materials represented by (probability) distributions of dielectric parameters in the polarization model [2]. We refer to the resulting model as the Maxwell-Random Lorentz model as now the polarization is a random process. Maxwell's equations are seen as coupled to the macroscopic polarization represented by the expected value of this random polarization.

The primary focus of the work is on a novel computational framework for such problems using Polynomial Chaos Expansions (PCE) as a method to approximate this improved model of polarization while allowing for easy simulation. PCE is a spectral in random space approximation method and exhibits exponential convergence for the expected polarization with respect to the number of terms in the expansion. As an example of a temporal and spatial discretization scheme that can be applied to this spectral model, we consider the popular Finite Difference Time Domain (FDTD) method. Stability and dispersion analyses are performed for the fully discrete scheme for the case of the second order Yee scheme in two spatial dimensions. We find that the stability condition for the deterministic model still holds for the random system, and the dispersion error exhibits exponential convergence.

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# Input-to-State Stability for Delayed Hybrid Systems and Application to $H_{\infty}$ Control System

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This paper addresses the problems of input-to-state stability/stabilization (ISS), and designing a robust reliable  $H_{\infty}$  control for a class of switched systems with state delay and time-varying, bounded disturbing input. The methodology of Lyapunov-Razumikhin (with multiple Lyapunov functions) is used to establish the ISS property. The importance of this method is that it provides delay-independent sufficient conditions to guarantee the ISS of the system modes, and later this result is applied to design the feedback  $H_{\infty}$  controller not only when all the actuators are operational, but also when some of them experience failure. The non-zero output of faulty actuators are treated as a disturbance signal that is augmented with the system disturbance input. The mode switching in the system is ruled by the general framework of average dwell-time (ADT) switching law.

The system under consideration has the form

$$\begin{cases} \dot{x} = f_{\rho(t)}(x_t, w(t)), \\ x_{t_0}(s) = \phi(s), \quad s \in [-r, 0], \quad r > 0, \end{cases}$$
(1)

where  $x \in \mathbb{R}^n$  is the system state and  $w \in \mathbb{R}^p$  is an input disturbance, which is assumed to be in  $L_2[t_0,\infty)$ , that is  $||w||_2^2 = \int_{t_0}^{\infty} ||w(t)||^2 dt < \infty$ . For all  $t \in \mathbb{R}_+$ , let x(t) be a function defined on  $[t_0,\infty)$ . Then, the delayed state  $x_t : [-r,0] \to \mathbb{R}^n$  is defined by  $x_t(s) = x(t+s)$  for all  $s \in [-r,0]$ , and its norm by  $||x_t||_r = \sup_{t-r \le \theta \le t} ||x(\theta)||$  where r > 0 is the time delay.  $\rho$  is the switching rule which is a piecewise constant function defined by  $\rho : [t_0,\infty) \to \mathscr{S} = \{1,2,\cdots,N\}$  where *N* represents the finite number of the system modes.

In using the method of Lyapunov-Razumikhin and to guarantee the robust global exponential ISS, we are led to solve a set of *N* algebraic Riccati-like equations for *N* positive-definite matrices,  $P_i$  for each  $i \in \mathcal{S}$ , by which the Lyapunov functions  $V_i(x) = x^T P_i x$  is defined. Also, under some conditions imposed on  $V_i$  along with the ADT switching law, we conclude that solution trajectory of the system is decreasing outside a certain neighbourhood of the disturbance function w(t).

The proposed results are enhanced by numerical examples with simulations.

# Solitary waves of a highly nonlinear fourth-order wave equation and their properties in different nonlinearity regimes

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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:

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

For this wave equation, all solitary wave solutions and all nonlinear periodic wave solutions, along with all conservation laws, are derived [5]. Several main results are obtained by parameterizing the solitary waves in terms of their wave speed and their asymptotic amplitude. First, the asymptotic amplitude is shown to be directly related to the continuum sound speed, and the ratio of asymptotic amplitude to peak amplitude is shown to describe the degree of dynamical nonlinearity in the underlying discrete system. Second, an algebraic relation is derived that determines the dynamical nonlinearity ratio in terms of the ratio of the solitary wave speed to the sound speed. In particular, highly supersonic solitary waves correspond to highly nonlinear propagating pulses in weakly compressed systems, and slightly supersonic solitary waves correspond to weakly nonlinear propagating pulses in strongly compressed systems. Third, explicit formulas for the physical height, width, impulse and energy of the solitary waves are obtained in both the strongly nonlinear regime and the weakly nonlinear regime. Finally, All cases in which the solitary wave expressions can be stated in an explicit analytic form using elementary functions are worked out.

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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# Using Cognitive Fit Theory to Evaluate the Effectiveness of Financial Information Visualization: An Example Using Data to Detect Fraudulent Transactions

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The main objective of this research was to investigate the impact that financial data visualization (DV) has on decision making for business related scenarios, specifically in detecting fraudulent transactions. This study addressed the following question: What effect does the financial DV format have on accuracy, speed, decision confidence, and memory retention associated with the completion of a task in detecting fraudulent transactions? DV could help to reduce the information volume to a manageable size, to focus on crucial data points, to gain insights, to draw conclusions by formulating theories on the basis of patterns, themes and calculations, to present and convey an effective message to stakeholders. The Cognitive Fit Model has been used in combination with prior literature in developing the hypothesis and research question. According to the Cognitive Fit Model (CFM) the effectiveness of the problem solving process is a function of the relation between the problem solving task and problem representation [3].

An experiment was designed to investigate the impact of DV on the outcome measures mentioned above. Research data was collected from experiments completed for this study. Participants were assigned to different groups. The study utilized three such groups, with each group presented with the same financial information in different formats: text/report, table and DV. Each group was asked to perform various tasks to assess their accuracy, speed of task, decision confidence, and memory retention. Participants for this research were business school students. For first stage of testing over 100 students participated. For next stage we are planning to include non-business students and business professionals.

This study focused on information presentation effects on a specific type of management judgment/decision making identification of possible fraudulent transactions. Fraud identification was selected due to critical importance of this issue. Data to create an experiment was based on data set using ACL (Audit Command Language) software. Benford's law [2] was used to create an experiment data to be reviewed by participants in order to find potentially fraudulent transactions. Effective data visualization has the potential for making the detection of fraudulent transactions more efficient and effective. Currently research of effectiveness of data visualization for fraud detection is limited [1]. DV could help to convert information to a manageable scope, identify and prioritize threats, develop critical intelligence and make effective decisions. DV can create the story behind the data, and in cases of potential fraud, can demonstrate linkages that are not obvious between people, places and financial and non-financial potentially fraudulent information.

The results of this study should be considered when designing decision making processes impacted by using different data presentation formats with focus in identifying potentially fraudulent transactions.

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### Measles: insights into waning immunity

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Measles is a vaccine preventable childhood infectious disease. However, every year new outbreaks are reported all over the world, even in countries achieving vaccination coverage levels at or above the target coverage of 95% [1]. It has been indicated that a cause of these cases may be related to the waning of vaccine-induced immunity [2,3]. We explore this using mathematical compartmental models (following *SIRV* framework with waning) describing measles dynamics and changes in immune status of individuals in a population, with and without age structure. Since the level of infectiousness of individuals that have waning vaccine-induced immunity is unknown, we vary this assumption in our studies. For the given model structure, we have derived the basic and control reproduction numbers ( $\Re_0$  and  $\Re_c$ ). We have also investigated how  $\Re_c$  is affected by changes in  $\Re_0$ , waning rates and the infectiousness of vaccinated individuals. Extending our study to a stochastic modelling framework, we have also quantified the probability of measles outbreaks in populations with specific  $\Re_c$ , and vaccine coverage and waning immunity rates. Briefly, we find that waning vaccine-induced immunity against measles can render measles elimination impossible. However, we also find that the probability of outbreak in highly vaccinated populations can be almost zero - meaning that elimination can be observed.

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### Proposed Decentralized IoT Security Solution Using Quantum Blockchain

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IoT (Internet of Things) security that ensures IoT devices will be cracked rapidly in the quantum-computing era quicker than we might suspect. Along this, Combining Quantum Computing and IoT is on interest because of its abilities. Quantum computing can help address the difficulties and issues that obstruct the development of IoT like Faster validation and verification process to its Applications for smart cities systems and frameworks like traffic, utilities, buildings, lights and health care. Quantum computing addresses that concern as it could accelerate the verification and validation process over every one of the frameworks to cooperate easily several times faster while guaranteeing steady enhancement of the systems. Confidentiality, integrity and authentication should be ensured for progressively secure communications Since IoT devices may contain sensitive data in which handling should conform to the rights and needs of users. Traditional security countermeasures and privacy enforcement cannot be directly applied to IoT technologies due to their limited computing power, moreover, the high number of interconnected devices arises scalability issues (1).

With the aid of quantum mechanics principals, we can provide high-secured communication using quantum cryptography, which uses algorithms that require more computing power than conventional PCs, for more complex against cyber-attacks using a practical application like post-quantum blockchain. Blockchain is an open, distributed ledger that can record transactions between two parties efficiently and in a verifiable and permanent way (2). Post-Quantum offers the ability to make your chosen blockchain quantum-safe (3).

The current IoT framework relay on a centralized network management architecture where there is a cloud server and all devices could be connected through it. Yet, in a decentralized Internet of Things framework, Blockchain could be an essential structure to make the transaction and participation of the devices very easy. Each device on the network works independently and combining that with quantum mechanics will guarantee that our proposed solution is secure today and tomorrow providing a safe transition to a new infrastructure for a smart quantum city, smart quantum home and smart quantum everything Because the entry of code-breaking quantum computers will be only a couple of years away.

In this paper, we will present a comprehensive survey of the current blockchain protocols for the IoT networks, summarizing the current overviews that deal with quantum blockchain technologies and propose a research development for iot security utilizing post-quantum blockchain. We provide quantum-safe signature schemes, supplanting the vulnerable public key cryptography currently used for validating and verifying transactions with lattice-based structure and apply it with IoT.

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# Development of a lattice Boltzmann model for the solution of partial differential equations

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Partial differential equations (PDE) are frequently encountered in modeling physical and industrial phenomena. To simulate these phenomena, robost, fast and efficient solution methods are required. There have been a lot of solutions techniques for different classes of PDEs. Traditionally, finite difference, finite volume and finite element methods have been used. However, the advances in computer technology and in particular, the emergence of multi and many core processors as well as graphic processing units (GPUs) and recent coprocessors demand more advanced PDE solvers which could employ all the available processing power on advanced computer hardwares.

The lattice Boltzmman method (LBM) has attracted many attentions in recent years as a recent efficient solution method for fluid flow simulations as well as general PDEs. Due to the local nature of the computations in the lattice Boltzmann method and its ease of programming, the LBM is an ideal candidate for developing efficient parallel PDE solvers suitable for recent computer hardwares.

In the present study, a recent lattice Boltzmann method, namely the central moment LBM has been used to develop an efficient PDE solver for transient heat transfer applications. The performance of this model is compared with that of the BGK lattice Boltzmann method as well as a traditional finite element based PDE solver. All these solvers have been developed using the Julia programming language which is a recent player amongst the scientific computing languages.

Several benchmark problems in transient heat transfer applications described by parabolic PDEs are solved and the results are compared with those of analytical solutions. It is shown that the the LBM could be used to solve PDEs accurately and efficiently and scales very well on recent parallel computer hardwares.

## An extended pseudo potential multiphase lattice Boltzmann model with variable viscosity ratio

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Multiphase fluid flows are important phenomena in industrial, scientific and engineering applications. However, their simulations could be very challenging for researchers. An efficient and recently developed computational fluid dynamic method for the simulation of multiphase flow is the pseudo-potential lattice Boltzmann method which has originally been proposed by Shan and Chen [1]. However, this model suffers from some limitations which have reduced its applicability for practical purposes. A literature review reveals that most researchers are using the same relaxation time for both phases in the pseudo potential model. It results in the kinematic viscosity of the phases being equal and the dynamic viscosity ratio is also considered to be equal to the density ratio [2, 3] which is not consistent with experimental data. According to the molecular theory the viscosity ratio is proportional to the density ratio but they are not exactly the same [4]. The coefficient of dynamic viscosity in a dense gas ( $\mu'$ ) is related to the corresponding coefficient in a normal gas ( $\mu$ ) by the following equation:

$$\frac{\mu}{\rho} = b\mu(\frac{1}{b\rho x} + 0.8 + 0.7614b\rho x) \tag{1}$$

By using Equation (1), one may find the viscosity ratio for different densities of fluids by:

$$\frac{\mu_1}{\mu_2} = n \frac{\rho_1}{\rho_2} \frac{\left(\frac{1}{\chi_1^h} + 0.8 + 0.7614\chi_1^h\right)}{\left(\frac{1}{\chi_2^h} + 0.8 + 0.7614\chi_2^h\right)} \tag{2}$$

where  $\chi^h = b\rho x$  can be determined from the compressibility of the fluid through  $\frac{dP}{dT}$ . To couple viscosity and density of the two phases to their theoretical values, it is feasible to utilize their Equation Of States(EOS).

Then, it would be feasible to link the viscosity of the two phases to the theoretical values calculated by the corresponding EOS as well as any other values which can be adjusted by the use of an extra factor n. The present numerical model is validated using two test cases: the static droplet and the two-phase Poiseuille flow. In these cases, the Laplace law test, the velocity profile, and the relative permeability prediction are investigated and compared with those of the analytical solutions. The results show that the suggested model enjoys the capability of changing the viscosity ratio as a function of the theoretical viscosity ratio and produce more physically based results.

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## Scatterer location via time reversal methods in acousto-elastodynamics

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Time reversal (TR) is a subject of very active research for over two decades. Many international teams are currently working on the subject from theoretical, physical and numerical points of view. It was experimentally developed by M. Fink in 1992 in acoustics [1], and showed very interesting features: a recorded signal, after passing through a barrier of randomly distributed metal rods, was refocus very precisely. The procedure is based on the reversibility property of wave propagation phenomena in non-dissipative media. As a consequence, one can "time-reverse" developed signals, by letting them propagate back in time to the location of the source (or scatterers) that emitted them originally.

Thenceforth on, numerous applications of this physical principle have been designed, in seismology, [2] or medical imaging [3]. Note however that, even if theoretically TR method should yield the exact solution, there is always the possibility that under some (realistic!) conditions - noise, partial information, lack of knowledge about the medium properties, etc.. - the time reversed process will fail.

In this talk, we propose to extend the TR method by considering acouso-elastic medium. This will help us to mimic for example breast tissue and to try to determine the scatterer location and property. Hence, we propose a method to identify an "inclusion", or to differentiate between two close inclusions, eventually with different elastic properties, corresponding to different breast tumors, for instance, benign and malignant. Basically, the method consists first in solving a forward problem to create synthetic (namely simulated) data recorded by receivers. From these data, one will solve a time-reversed problem to compute a reversed field. Then, in the same spirit as in reverse time migration or topological gradient methods, one will correlate this forward and backward responses in time to construct an imaging function. Using the intersection of these two wave fronts will help us to determine the inclusion location and some of its properties.

In addition, to be closer to what happens in many real cases as in medical imaging and other fields, we do not assume that the line of receivers encloses the bounded domain  $\Omega$ , we rather consider that the aperture is reduced, and that only noisy data are available. For the sake of simplicity, we will consider a "layered" medium and we want to determine the presence of "inclusions" in the elastic part, from recorded acoustic waves scattered by these inclusions. However, the method does not require *a priori* knowledge of the physical properties of the inclusions.

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## **Explicit-Implicit SDP Relaxation Scheme in Combinatorial Optimization**

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It is widely considered that the *semidefinite programming* (SDP) methods [1] gained an increasingly growing popularity upon the time when important and unprecedented results on certain combinatorial optimization problems were obtained. However, scrutinizing the available literature indicates that many of those groundbreaking results were achieved only for a limited classes of combinatorial optimization problems such as *maximum cut, maximum stable set* and *graph coloring* problems [2]. Moreover, the vast majority of such prominent works relied mainly on the use of the so-called *Shore's semidefinite relaxation scheme* [1]. We first investigate the circumstances under which employment of such a relaxation scheme leads (or fails to lead) to promising results.

In this work, we gear our focus towards discrete combinatorial optimization problems in which the SDP relaxations are utilized within *branch-and-bound* or *branch-and-cut* methods [3] for the purpose of deriving bounds on the integral objective values. In such applications, one would often desire to add a set of valid constraints (cuts) to the relaxed model in order to strengthen the quality of the bounds obtained. However, for many combinatorial optimization problems, complexity of their feasible regions usually renders formulation of such valid cuts difficult, if not impractical. To overcome those challenges, we develop a two-stage SDP relaxation approach which we refer to as the *explicit-implicit relaxation scheme*.

More precisely, in explicit stage of our developed scheme, the typical Shore's semidefinite relaxation is employed, yielding an optimal solution in the form of a positive semidefinite matrix. Thereafter, in the implicit stage, the obtained solution of the former stage is utilized to generate a set of promising positive semidefinite matrices which can potentially strengthen the bound obtained by resorting to Shore's semidefinite relaxation method. It is noted that the term *implicit* is employed, in that each generated positive semidefinite matrix is associated to a SDP model whose underlying structure is not explicitly given.

As an application, we consider one-dimensional 0-1 knapsack problems in which a subset of items has to be assigned into a knapsack of a given capacity. Once the problem is formulated as a SDP, the Shore's relaxation is obtained in the explicit stage of our developed scheme. Then, we opt to employ Wishart distribution in order to generate the positive semidefinite matrices pertaining to the implicit stage. More specifically, the optimal matrix derived in the explicit stage is fed into the Wishart distribution as the scale matrix, and subsequently the promising matrices are generated using Monte Carlo method. Our computational results show that the proposed relaxation scheme is indeed effective to tighten the bound.

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## **Coulomb Explosion Imaging: Super-resolution by Optical Properties of Electrostatics Lens**

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A velocity map imaging (VMI) is a popular technique in a Coulomb explosion imaging experiment with the capacity to focus photo-fragments based on their initial velocity vectors. The VMI is capable of achieving this feat as a result of the system of electrostatic lenses (also known as electrodes) with varying potential, which the photo-fragments have to transit. However, despite the focusing capability of the VMI, the measured time-of-flights of the photo-fragments still suffer from a temporal spread, which is a consequence of the initial velocity and spatial spread at the point of formation.

To be able to reconstruct the states of these photo-fragments at the point of formation, there is a need for a better understanding of how the system of electrostatic lenses alter the trajectories of the photo-fragments between formation and detection to achieve a velocity-map. This talk will cover the concepts of VMI, modelling and asymptotic analysis of the systems of electrostatic lenses and how the understanding of the impact of the system of lenses on the fragment trajectories can reduce spatial spread.

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## Choosing between non-mutually exclusive social groups

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Suppose that agents are offered by a planner many variants of the same good or service. Agents have dichotomous preferences over these variants: a variant is acceptable or it is not. Agents self-report these preferences. By selecting a given variant, the planner thus makes winners out of the agents finding that variant acceptable. Hence, from the point of view of the planner, choosing a variant is akin to choosing among non-mutually exclusive groups. Examples of such settings include the selection of the time slot for a group event, the location of a public good, where agents might approve multiple locations (i.e. anywhere near my commute), the specifications of a public good or public policy, where agents might favor different quality/tax trade-offs, opening hours for a governmental office, with agents agreeing with hours that they find convenient, the restaurant/type of cuisine for a group meal or the subfield of economics that will be prioritized in a grant competition (or in a search to fill a new position).

Approval voting, which selects (possibly a subset of) the variants that are acceptable to the most agents, could be a solution here. However, because the applications we have in mind are not about electing a candidate, but rather about utilizing common resources, we argue that this is not the only interesting mechanism. Consider an example where the agents are a, b, c, d and there are 4 variants available. Suppose that the first variant is acceptable to a and b, the second to a and c, the third to a and d, and the fourth to b, c and d. Notice that agent a is not being difficult: he finds acceptable three of the four variants, while every other agent only finds two variants acceptable. Yet, if the most popular variant (the fourth one) is chosen then agent a is shut out. This simple example shows that approval voting is not necessarily fair: agent a is the most flexible, but he is just unlucky that no more than one of his colleagues share his acceptance of a variant (something he has no control over). There is thus a clear conflict between efficiency and fairness in this context. More generally, pushing the idea that agents are not responsible for the preference of others, a legitimate objective of the planner could be to try to give everybody an opportunity to win.

This objective can be combined with a minimal Pareto-Efficiency criterion stating that if a group is a subset of another group that could also be selected, then we should never choose the subset. An additional consideration is asymmetric information, as agents could misrepresent their preferences to increase their odds of obtaining an acceptable variant. We thus aim to find methods that are Strategy-Proof in the sense that agents find it best to reveal their actual preferences. We also consider properties of fairness and coherence.

We build ranking-based methods that satisfy our properties in the following way: we first fix a ranking of all possible coalitions of the agents and the planner simply selects the highest ranked among those generated by the preference revelation. We show that the properties on the methods are linked to the properties of the ranking used. To obtain a ranking-based method that satisfies Pareto-efficiency and Strategy-Proofness, we need the ranking to be inclusive: if  $S \subset T$ , then T is ranked above S. An additional property is Independence of Ubiquitous Agents: if an agent belongs to all Pareto-efficient coalitions, we should be able to remove her from the problem without changing the chosen probabilities. We obtain this property if the ranking leads to a biased result in favor of the coalitions preferred according to the ranking, averaging over rankings allows to make the method unbiased. We show how to obtain unbiased ranking-based methods that satisfy all of our properties, differing on their ability to select only maximal-approved coalitions or any Pareto-efficient coalitions.

## Machine Learned Exchange-Correlation Functionals in the GPAW Environment

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Kohn-Sham density functional theory (DFT) is a computational method that is used for modelling the electronic structure of interacting atomic systems. The mathematical basis for DFT is the Hohenberg-Kohn Theorem, which guarantees the existence of a one-to-one mapping between the ground state electron density of system and its external potential. It follows that the quantum *N*-body problem (which classically requires finding a wavefunction of 3*N* variables) can be solved by finding the ground state electron density, a function of 3 variables only.

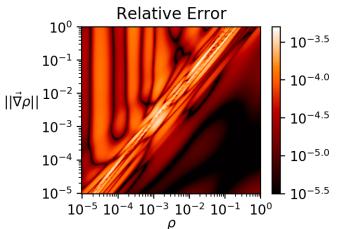


Figure 1: Plot of the relative error in the XC energy density for a neural network trained on the PBE [2] functional, where  $\rho$  is the electron density in atomic units. The error is greatest along a diagonal strip, where the PBE functional transitions between the slowly and rapidly varying density limits.

A necessary ingredient for any DFT calculation is the *exchange-correlation* (XC) functional, a mapping that relates the ground state electron density of a system to its total energy. However, the exact form of the XC functional is unknown, and it has remained an open problem to find this functional since the birth of Kohn-Sham DFT in the 1960s. At present, any DFT calculation must approximate this unknown functional, necessarily leading to an error that can be large and difficult to quantify. Many approximate XC functionals have been proposed and are in use, but none are universally valid for every atomic system.

The seemingly intractable nature of the exact XC functional suggests employing *artificial neural networks* (ANNs) for building approximate XC functionals. An NN XC functional offers the possibility of systematic improvement, as by training on more data an NN can learn increasingly complex behaviour and yield greater accuracy. In this work, we have implemented a variety of approximate XC functionals using NNs, and interfaced these networks with the GPAW [1] DFT environment. We discuss the performance of these networks and pos-

sible routes for improvement. The possibility of training a non-local NN XC functional is of particular interest, as such a functional could greatly improve upon current approximations. We discuss how we are approaching this problem and the difficulties we are facing.

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## A Model for the Binary Asteroid 2017 YE5

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The asteroid 2017 YE5, first discovered in December 2017, was determined in June 2018 to be a rare binary pair of asteroids with an even more rare property of the two asteroids having nearly equally masses. We propose a simplified four-body problem for the motion of a binary pair of asteroids of arbitrary but small masses in the presence of two primaries of larger masses whose motion is independent of the binary pair of asteroids. We investigate numerically and analytically the existence of geometric structures in phase space that lead to the separation of the two asteroids in a "tight" binary pairing. We further investigate the possible behaviours of the two asteroids after separation, i.e., capture of one asteroid by a primary, ejection of the other asteroid far from the primaries, etc.

## **Dispersive Equations with Random Time-dependent Potentials**

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In this talk I shall present recent results about evolution equations with time-dependent random potentials.

## **Rationality and Stability in Bargaining Games Played by Finite Automata**

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Aspects of behavioral decision-making can be integrated into game-theoretic models of two-player bargaining using finite automata to represent bargaining strategies [2, 1]. Empirically observed bargaining and decision-making heuristics can then be implemented into these strategy sets to form quasi-rational bargaining automata. The automata are used as bargaining agents who must jointly agree upon a fixed allocation of transferable utility in an infinite-horizon Rubinstein bargaining game [3]. At each turn, the automata are given the opportunity to accept a proposed portion of the transferable utility, or to reject the proposal and make a counter-offer of their own. The bargaining game will continue until an agreement is reached and each player receives their agreed upon portion of transferable utility.

The meta-game analysis looks at how a player would select an automaton as his bargaining agent, given different bargaining situations. A range of different simulations were performed, analyzing the overall bargaining effectiveness of different populations of automata. In addition, the outcomes for the individual player and the entire group of players are assessed for their efficiency and fairness. The equilibria in the meta-game are used to propose a bargaining model to be tested empirically.

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## New Classes of Potentials with Exact Eigenvalues and Eigenfunctions J. Benbourenane<sup>1</sup>

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It is well known that exact solutions of the Schrodinger equations are limited to few known potentials and due to this fact all the physical quantum system will try to model the potentials to one of these known potentials or use approximation methods to take advantage of them. Supersymmetry is one of the powerful techniques to determine the energy and the wave functions of quantum systems with defined superpotentials.

The use of Supersymetric Quantum Mechanics (SUSY-QM) technique and shape invariance will allows us to completely determine the spectrum of a quantum system. In this talk, exact solutions to the Schrodinger equation are obtained where the eigenvalues and eigenfunctions of new defined classes of potentials, with partner potentials written as linear combinations of a set of linearly independent hyperbolic functions, such corresponding potentials could be used as good models in quantum physics and molecular chemistry.

#### The effect of two delays on stability of the Mackey-Glass equation

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The presence of several delays instead of one delay can create a new type of dynamics: an equation which was stable for coinciding delays can become unstable, once the two delays are different, creating sustainable oscillations. The maximal delay value will influence the oscillation amplitude.

The Mackey-Glass equation

$$\dot{x}(t) = r(t) \left[ \frac{ax(h(t))}{1 + x^{v}(h(t))} - x(t) \right]$$

was introduced in [1] and investigated in [2], see also the review of results in [3].

The situation when the same production function involves different delays is quite common in real-world models. Two types of delays occur, for example, in gene regulatory systems where the translation delay and transcription delays involved in the function significantly differ. If the Mackey-Glass equation

$$\dot{x}(t) = r(t) \left[ \frac{ax(h(t))}{1 + x^{\nu}(g(t))} - x(t) \right]$$

with a > 1 and v > 0 incorporates not one but two variable delays, some new phenomena arise: there may exist non-oscillatory about the positive equilibrium unstable solutions, the effect of possible absolute stability for certain *a* and *v* disappears. We obtain sufficient conditions for local and global stability of the positive equilibrium and illustrate the stability tests, as well as new effects of two different delays, with examples.

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## **Traffic Dynamics Subject to Random Misperception**

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There is a tremendous amount of research on safety of automotive technology – nowadays, especially concerning the development of autonomous vehicles. Still, the benefits of traveling require that one tolerates a small amount of downside risk: traffic accidents may occur. In this talk, we present a traffic model which incorporates the possibility of errors and, thus, allows to study the tradeoff between safety and efficiency for various traffic systems.

Among traffic models, *car-following models* describe the movement of vehicles on a microscopic level. Here, velocity and acceleration of each vehicle on a one-lane road are governed by an ordinary differential equation which is coupled to the motion of the preceding vehicle. Typically, these models are accident-free. In [1], an extension of such a car-following model (more precisely, of the Intelligent Driver Model, cf. [2]) is proposed which introduces perceptional errors modeled by stochastic processes (e.g., Ornstein-Uhlenbeck processes). Simulations show that such errors accumulate over time and lead to accidents. Technically, we transform each ordinary differential equation (RODE). We explain how this approach can be generalized to model more complex scenarios such as intersections where additional conflicts arise (cf. [3]). Moreover, we discuss how the  $\gamma$ -RODE-Taylor scheme (cf. [4]) can be employed to obtain approximate solutions to our model.

We characterize traffic systems in case studies by means of Monte Carlo simulations. For this, we evaluate different performance measures which we relate to safety margins and error sizes.

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## How to compute ideal class groups using subfields

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We present an algorithm that computes the ideal class group of certain families of number fields by recursively performing this task in subfields. In families of real multiquadratic fields, the computation of the ideal class group derives from *S*-unit groups in quadratic subfields. The resulting complexity can be as low as polynomial in the discriminant of the input multiquadratic number field. We implemented our algorithm and we were able to compute ideal class groups of multiquadratic fields of degree up to 128 on a single core. Finally, we discuss how to extend this recursive approach to wider classes of number fields.

## Computing the Regulator of a Real Quadratic Order Using p-Adic Methods

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The regulator of a real quadratic order  $\mathcal{O}_K$  is defined as  $\log \varepsilon$ , where  $\varepsilon$  is the fundamental unit of  $\mathcal{O}_K$ . The coefficients of the fundamental unit can become very large, so rather than directly compute the regulator from  $\varepsilon$  we typically use a power product representation of units derived from a generating set of relations for the class group of  $\mathcal{O}_K$ . Existing methods for computing the regulator from this data suffer from a variable loss of precision which can be difficult to control. We propose a p-adic method which simplifies the management of the precision throughout the computation. We implement the new method in C++ and compare the performance with that of existing implementations.

## **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:

$$Kf(x) = \int_{a}^{b} k(x, y)f(y)dy = g(x),$$
(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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## **Optimal Control in Fluid-Elasticity Interactions**

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We consider optimal control problems subject to moving boundary fluid-structure interactions (FSI). FSI are ubiquitous in medical and engineering applications, ranging from blood flow in stenosed arteries and heart valve dynamics to the design of small-scale unmanned aircrafts and morphing aircraft wings. Some problems of interest consist of (i) minimizing turbulence in blood flow inside a stenosed or stented artery, (ii) controlling the behavior of the FSI to achieve a given target fluid velocity or pressure, or (iii) minimizing the hydro-elastic pressure on the interface between the two environments.

FSI are highly nonlinear couplings of parabolic-hyperbolic type, described by a mismatch of regularity of the two solutions at the common interface. First, we present a global well-posedness result for the system with small distributed sources. Then we discuss the existence of optimal control for the problem of minimization of drag in the fluid.

## Modelling Bike Sharing Systems with Dynamical Systems

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Various large cities throughout the world create Bike Sharing Systems (**BSS**) where customers can rent a bike at one station and return it at a dock in another. This creates problems for the renting firm as the amount of bikes and the amount of empty docks available at stations vary throughout the day and week. As a result, the system will often require rebalancing within a day or throughout the week. Modelling a modern BSS appropriately and using the model correctly to predict which stations to increase the number of docks or bikes at can greatly reduce the need for rebalancing the network.

We propose a discrete dynamical system model for a BSS to study clustering, stability, sensitivity, and transition dynamics. Simulation techniques and real-world data are applied to model development, testing, and evaluation. We also study clustering criterion for the stations based on location and transactions. Some results on system optimization are discussed.

## Natural Subsystems in a Biochemical Reaction System with Multiple Steady States and Hysteresis

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Systems biology seeks to develop new mathematical methods for analysing genetic regulatory and metabolic pathways [1]. Edelstein [2] introduced a simple biochemical model with multiple steady states and hysteresis. Methods from algebraic geometric and convex analysis are increasingly used for studying the dynamics of this and similar biochemical reaction networks (e.g., [3, 4]). On the other hand, any biochemical reaction system can be modelled using a canonically derived Petri net [5] and functorially associated automata [6]. Such discrete event dynamical systems, in which different events (reactions), can occur in arbitrary sequences can be analysed using Krohn-Rhodes algebraic automata theory and transformation semigroup theory [7, 8]. This approach identifies hierarchical structure of natural subsystems with locally reversible dynamics. These natural subsystems comprise maximal subgroups of the discrete dynamical system's transformation semigroup and act on the image of an idempotent element  $e^2 = e$ , the identity of the subgroup, which collapses the state space onto its image [8]. Edelstein's biochemical reaction system is given by 5 abstract chemical species and 3 pairs of reactions:

 $A + X \rightarrow 2X, X + E \rightarrow C, C \rightarrow E + B$ and their reverse reactions,

where each of the 6 reactions occurs according to mass-action kinetics with a particular reaction specific rate constant. Trajectories of the state of this system preserve the invariant quantity given by #A + #B + #E + #X + 2#C as each reaction leaves it unchanged. We describe the structure of the transformation semigroups for fixed values of this invariant using computational Krohn-Rhodes decompositions techniques [6, 9] applied to the Petri net of Edelstein's reaction network, study the permutation group structures that arise in its natural subsystems, and seek to relate these to the biochemical system's multiple steady states and its hysteresis properties.

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## **Comparing Regularization Techniques Applied to a Perceptron**

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Overfitting is a common problem that is faced when dealing with neural networks, especially as computers continue to get more powerful, and we have the capability to train larger networks with many free parameters. As a result there is a pressing need to develop and explore different techniques to reduce overfitting; an extremely popular and important area of current work within the deep learning community.

Current research [1] suggests that regularization can help to avoid overfitting a neural network and improve how it handles new and unobserved data. For example, [2] illustrates that an  $L_0$  regularization approach smoothes a network model and accelerates its training. Such an approach can be extended to other types of networks beyond traditional Artificial Neural Networks (ANN) such as Convolutional Neural Networks (CNN) and Interval Neural Networks (IANN), which are both important topics in deep learning. In this talk, we will discuss the single perceptron model and do a quantitative comparison of two commonly used regularization techniques,  $L_1$  and  $L_2$ , added to the model. Finally, we will present plans for applications to real data and future work involving related and hybrid techniques.

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## Domain decomposition based preconditioning for the integral equation formulations of the forward and inverse scattering problem

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We propose domain decomposition preconditioners for the solution of an integral equation formulation of the forward and inverse acoustic scattering problems with points scatterers in two dimensions. We study independently both problems and propose preconditioning techniques to accelerate the iterative solvers.

In the forward scattering problem, given a collection of point scatterers **q** and an incident wave  $u^{inc}$ , we solve the Lippmann-Schwinger Equation to obtain the value of the scattered field  $u^{scat}$  [1]. For **q** formed by N point scatterers, we solve an  $N \times N$  dense linear system of equations. To speed-up the solution of this system, we extend the domain decomposition based preconditioning techniques presented for partial differential equations in [2] to integral equations. We combine this domain decomposition preconditioner with a low-rank correction, obtained by a randomized algorithm [3], forming a new preconditioner.

In the inverse scattering problem, we seek an approximation  $\tilde{\mathbf{q}}$  of the unknown true scatterer  $\mathbf{q}$  given measurements  $u^{meas}$  of the scattered field. This problem is nonlinear and ill-posed. We use the Gauss-Newton method for the nonlinearity and Tykhonov regularization for the ill-posedness. At each step of the Gauss-Newton iteration we solve a dense linear system of equations using an iterative method. To improve the speed of convergence of the iterative method, we use the low-rank corrected preconditioner proposed for the forward problem as the building block for constructing a preconditioner for the Gauss-Newton Hessian.

For both problems, our numerical results show that both preconditioning strategies work well. In particular, for the inverse scattering problem, our preconditioner outperform low-rank approximations.

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## Persistence in Firm Growth: an Inter-Distributional Analysis

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What is the degree of persistence in firm growth? Does *success brings success*, as recently expanding firms have a higher probability to achieve sill higher market shares or, conversely, a mean-reverting effect is in place, ultimately equalizing the observed growth rates of different firms over multiple years? Answers to this question has been traditionally limited to discussing the sign and significance of the one-lag coefficient in a possibly augmented autoregressive growth model. We maintain that the widely heterogeneous nature of firms and of their growth patters cannot be captured by such simplistic linear models. Thus, in this study, we approach the analysis of firm growth persistence from a wider perspective, exploiting intertemporal mobility in the intra-distributional rankings of firm growth rates. Using a panel of Italian manufacturing firms over the period 2009-2017, we study the transition matrix (TPM) between the deciles of the growth rate distributions is successive years. An example of the kind of matrix obtained is reported in Figure 1. If the linear autoregressive model were sufficient, we should find a homogeneous behavior across all initial size classes (columns). As can be seen, this is not the case: the process displays some degrees of persistence for moderate growth rates, while a mean-reverting effect is noticeable for extreme growth events. Overall, the degree of persistence measured using standard mobility measures is low (Shorrocks=0.9510, and Bartholomew=0.3445). In order to perform a systematic application of this analysis across countries and sectors, two difficulties must be overcame. First, the analysis resting on the Markovianity assumption, it is necessary to establish the degree of stationarity of the firm growth process. We apply a standard  $\chi^2$  test to assess whether all the underlying pairwise TPMs are indeed homogeneous. Results in Table 1 show that the null of homogeneity is generally rejected. This might be due to the relation of growth rates with firm size. Indeed the presence of a negative exponential scaling between variance of growth and firm size is a well documented fact on these data. In this respect, we plan to repeat the TPM analysis on suitably defined residuals of an auxiliary non-linear regression model that accounts for the observed heteroskedasticity. Second, we need to develop new synthetic indexes of persistence able to better capture the peculiarity of the firm growth process. The literature on TPM-based measures of persistence is almost entirely developed with macro-economic variables in mind, that is for processes that are smoother and more homogeneous that those observed at the level of individual firms.

Years compared	$\chi^2$	d.o.f	p-value
(2010/2011) (2011/2012)	276.206	90	0.000
(2011/2012) (2012/2013)	118.177	90	0.025
(2012/2013) (2013/2014)	105.290	90	0.129
(2013/2014) (2014/2015)	94.420	90	0.354
(2014/2015) (2015/2016)	133.339	90	0.002
(2015/2016) (2016/2017)	105.041	90	0.133
All pairwise transitions	1126.108	540	0.000

Table 1:  $\chi^2$ -square test of TPM homogeneity

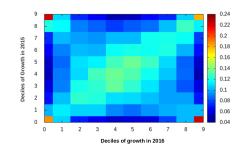


Figure 1: TPM in growth 2015/2016 for Italy

## Defining the Planck Constant: the link between microscopic quantum measurements and macroscopic masses

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The scale parameter for quantum mechanics is Planck's constant h [1]. The most accurate measurements of h have been based on the use of Kibble balances [2] operating with macroscopic masses. The circumstances are now so much improved that the process has been inverted; henceforward, Planck's constant will be an exactly defined quantity, and Kibble-type balances will be used to realize the kilogram standards [3]. An analogous redefinition of the macroscopic metre standard took place earlier, enabled by advances in quantum-based atomic clocks.

Defining Planck's constant will provide a direct link between microscopic quantum measurements and macroscopic masses. In the Kibble balance scheme for realizing the future "electronic kilogram", the macroscopic mass m is linked to the Planck constant by the equation

$$m = hnf_1 f_2 / 4vg \tag{1}$$

where *n* is an integer,  $f_1$  and  $f_2$  are two precisely measured microwave frequencies, *v* is the speed with which the Kibble balance coil moves in the magnetic field and *g* is the local value of the acceleration due to gravity.

The superconducting watt balance is one proposed implementation of the Kibble balance scheme which is particularly intriguing [4]. By eliminating the DC resistance R of the moving coil, the moving phase and weighing phase of the watt balance can be combined without having to correct for the Ohmic voltage drop IR. This would be a much more elegant measurement scheme than current Kibble balances allow. The superconducting moving coil watt balance would provide a direct link between the macroscopic mass m and microscopic quantum measurements, and is therefore highly useful as an archetype of a real-world measurement of a macroscopic object, which nonetheless depends explicitly on quantum mechanical parameters. In this talk I will discuss various implications of a superconducting watt balance scheme for the realization of macroscopic masses, and some of the engineering challenges.

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## The Excess Method: A Multiwinner Approval Voting Procedure to Allocate Wasted Votes

Steven Brams, New York University Marcus Brill, Technische Universitat Berlin

In using approval voting to elect multiple winners to a committee or council, it is desirable that excess votes-approvals beyond those that a candidate needs to win a seat-not be wasted. The excess method does this by sequentially allocating excess votes to a voter's as-yetunelected approved candidates, based on the Jefferson method of apportionment. It is monotonic-approving of a candidate never hurts and may help him or her get elected-computationally easy, and less manipulable than related methods. In parliamentary systems with party lists, the excess method is equivalent to the Jefferson method and thus ensures the approximate proportional representation of political parties. As a method for achieving proportional representation (PR) on a committee or council, we compare it to other PR methods proposed by Hare, Andrae, and Droop for preferential voting systems, and by Phragmén for approval voting. Because voters can vote for multiple candidates or parties, the excess method is likely to abet coalitions that cross ideological and party lines and to foster greater consensus in voting bodies.

#### GLOBAL SOLUTIONS OF THE COMPRESSIBLE NAVIER-STOKES EQUATIONS

#### CHENG YU

In this talk, I will talk about the existence of global weak solutions for the compressible Navier-Stokes equations, in particular, the viscosity coefficients depend on the density. Our main contribution is to further develop renormalized techniques so that the Mellet-Vasseur type inequality is not necessary for the compactness. This provides existence of global solutions in time, for the barotropic compressible Navier-Stokes equations, for any  $\gamma > 1$ , in three dimensional space, with large initial data, possibly vanishing on the vacuum. This is a joint work with D. Bresch and A. Vasseur.

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#### Generic structure and stability of solutions to Stackelberg games

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Abstract. We consider a non-cooperative game with a leading player that announces his strategy in advance, and a follower who implements the best reply to the leader's action. For an open, everywhere dense set of  $C^3$  cost functions to the follower, we provide a detailed description of the qualitative structure of the best reply map. In turn, for a generic  $C^2$  cost function to the leader, we show that the Stackelberg equilibrium is unique. Moreover, it is stable w.r.t. small perturbations of the two costs. The main proofs rely on Sard's theorem and on Thom's transversality lemma.

## **Detecting Square Numbers in Binary Arithmetic**

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We will discover some facts about the digits of square numbers (perfect squares) if they are expressed in a base which is a power of 2, for instance octal or hexadecimal arithmetic and present an algorithm in binary arithmetic for testing whether or not a natural number *N* is a square number and/or computing its square root, with time complexity of  $O\left(\frac{\log^2 N}{s}\right)$  where *s* is the power of the chosen base (i.e. s = 3 for octal arithmetic, s = 4 for hexadecimal arithmetic, etc.).

The algorithm builds up the square root of a number (if it exists) from the low order digits to the high order digits whereas algorithms which use Newton's method or simple binary search (for example sieve methods) find the higher order digits first.

The following lemma and theorems provide the theoretical basis for the algorithm (in octal arithmetic).

**Lemma 0.1.** If j, k are odd and  $j^2 \equiv k^2 \mod 8^l$ , then either  $j + k \equiv 0 \mod \frac{8^l}{4}$  or  $j \equiv k \mod \frac{8^l}{2}$ .

**Theorem 0.2.** If N is odd and  $N \equiv 1 \mod 8$ , then for each positive integer l there exists a unique odd number  $k_l$ , with  $k_l < 8^l/4$ , such that  $k_l^2 \equiv N \mod 8^l$ . Furthermore:

- (i) The numbers  $k_l$  form an increasing sequence (i.e.  $k_l \le k_{l+1}$  for each l) and, if  $k_l \ne k_m$  for l < m, then  $k_l < 8^l/4 < k_m < 8^m/4$ .
- (ii) If N is a square number then (for each l) we have  $N = \left(\frac{8^l}{2}p_l \pm k_l\right)^2$ , where  $p_l$  is the unique nonnegative integer such that  $\frac{8^l}{2}p_l 8^l/4 < \sqrt{N} < \frac{8^l}{2}p_l + 8^l/4$ .

**Theorem 0.3.** If  $N \equiv 1 \mod 8$  and its octal expression has 2m or 2m - 1 digits, and the odd numbers  $k_l$ , for  $l \leq m+1$ , have the properties stated in Theorem 0.2, then N is a square number if and only if one of the following statements is true.

- (i)  $N = k_{m+1}^2 = k_m^2$ (ii)  $N = k_{m+1}^2 = (\frac{8^m}{2} - k_m)^2$ (iii)  $N = k_{m+1}^2 = (\frac{8^m}{2} + k_m)^2$
- (*iv*)  $N = k_{m+1}^2 = (8^m k_m)^2$

## Simulating coherent electron shuttling in quantum dots

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Coherent transport of electron spins is required for several proposed large-scale architectures based on quantum dot spin qubits [1, 2]. In [1], spin singlets are distributed across neighboring computational nodes by sequential single-electron tunneling through a linear array of quantum dots. We adopt a simplified metal-gate geometry for silicon MOS dots and use the nextnano++ software to determine the potential landscape as a function of varying gate voltages (an example device geometry and typical simulated potential is shown in Figure 1a). The extracted potential landscapes are subsequently used when solving the time-dependent Schrodinger equation in 1D to simulate coherent electron shuttling. An algorithm, based on satisfying the adiabatic criterion, is presented that calculates time-dependent voltages that maintain a desired fidelity with the ground state orbital wave function. These tools are used to vary the geometrical device parameters to maximize the electron shuttling velocity and extract what tunnel coupling strengths can realistically be achieved. We further show that the essential physics can be captured in an effective Hamiltonian model, which allows us to explore how spin-orbit and valley states affect the shuttling fidelity and maximum velocity when shuttling an electron from an spin-entangled electron pair. We find ranges for the effective Hamiltonian parameters that allow for high fidelity and fast shuttling and compare whether they are realistically achievable based on experimental data.

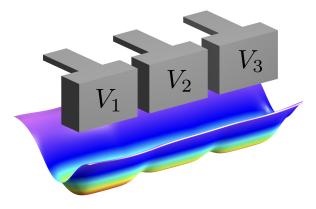


Figure 1: A 3D schematic of the simplified gate geometry (grey structure) for a linear quantum dot chain. The structure is modelled in nextnano++ to extract the potential landscape (plotted in color) for a given set of gate voltages  $\{V_1, V_2, V_3\}$ .

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## Invariant tori for a class of singly thermostated hamiltonians

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A thermostated hamiltonian system models a hamiltonian system that is immersed in a heat bath. A fundamental question about such a system is whether it reaches statistical equilibrium with the heat bath. Even for 1-degree-of-freedom hamiltonians this question is non-trivial, and an answer has only been known in the simplest case by work of Legoll, Luskin and Moeckel [4, 5].

In this talk, I will give a mathematical definition of a thermostated hamiltonian system and show how the properties of the system lead to the existence of a thermostatic equilibrium when the thermostat is only weakly coupled with the hamiltonian. Under a modest additional hypothesis on the non-degeneracy of this equilibrium, one obtains the existence of invariant tori in a neighbourhood of the equilibrium.

As an application, it is proven that if the hamiltonian is real-analytic and "well-behaved" and if the thermostat is one of four well-known examples in the literature [1, 2, 3, 7, 8], then these invariant tori exist for all but finitelymany temperatures.

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## **Modeling Open Quantum Systems**

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Modeling open quantum systems is a difficult for many experiments. A standard method for modeling open system evolution uses an environment that is initially uncorrelated with the system in question, evolves the two unitarily, and then traces over the bath degrees of freedom to find an effective evolution of the system. This model can be insufficient for physical systems that have initial correlations [1]. Unfortunately, there is no known method of modeling an open quantum system which is completely general [2]. Here we discuss some work to describe the evolution more generally using affine maps of the polarization vector, and dynamical maps that are not completely positive [3]. We then discuss some implications a more general treatment would have for quantum control methods [4].

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## Advances in the forensic estimation of time of death

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The field of forensic science works closely with entomologists to estimate time of death when pathological information is no longer available. Within the first two to three hours of the body's exposure blow flies and house flies will colonize the body [1]. These insects are involved in the decomposition of the body and so analysis of their development is required for a minimum post mortem interval (PMI) estimate.

Since development through the life cycle of insects is driven by the ambient temperature [3], the temperature profile at the scene, prior to its discovery, is required to characterize the rate of development of the insects. Current methods use two temperature profiles to create a predictive equation to extrapolate previous temperatures.

We find some inaccuracies in this method. We propose a mathematical model for temperature prediction that combines environmental coupling effects as well as the presence of heat sources or sinks [2]. We choose to use a simplified heat equation that combines these effects, modelled by

$$\frac{\mathrm{d}\bar{T}}{\mathrm{d}t} = c(T_0(t) - \bar{T}) + s \quad \text{with} \quad \bar{T}(0) = \bar{T}_{\mathrm{meas}}(0), \tag{1}$$

where  $\overline{T}$  represents the temperature at the scene,  $T_0(t)$  is the temperature at the weather station, *c* represents the coupling between the body and its environment and *s* represents the source term which are assumed to vary slowly in time. In this application the source will typically be a positive real number to represent the heat of decay on the body. It is important to note that while working with case study data we have chosen the initial condition to be a known value recorded at the scene, however in practice this will not be available.

Upon comparing the generated temperature profiles of the two models, we see that the simplified heat equation is more accurate and is able to include more information about environmental conditions. We hope that with improved methods for temperature predictions, a more informed and precise PMI estimate may be made.

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# Using shooting approaches to generate initial guesses for ODE parameter estimation

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We consider the parameter estimation problem for parameterized systems of ordinary differential equations (ODEs). This problem involves finding the set of parameters that best fit a set of observed data. In particular, we consider techniques for generating initial guesses that are close to the best fit parameters, such that a shooting approach is likely to converge. We discuss approaches used in the literature and demonstrate how they can be improved using ideas motivated by progressive and multiple shooting. The presented approaches are then applied to a test problem from the literature.

## Formal stability of L<sub>4</sub> in the spatial restricted circular three-body problem

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In this talk we present some new results on the well-known problem of the nonlinear stability of  $L_4$  and  $L_5$  in the spatial restricted circular three-body problem.

In the framework of nonlinear stability of elliptic equilibria in Hamiltonians with n degrees of freedom we provide a criterion to obtain a kind of formal stability called Lie stability [7]. Our result generalises previous approaches as, for instance, exponential stability in the sense of Nekhoroshev (in most of the cases). In case of formally stable systems we bound the solutions near the equilibrium over exponentially long times [4]. To our knowledge there are no examples of systems that are formally stable but not Liapunov stable, which gives an idea of the strength of formal stability in the setting of nonlinear stability of equilibria.

Surprisingly there is almost no connection in the literature between Nekhoroshev stability of elliptic equilibria and formal stability. Indeed, excepting the pioneering papers by Glimm [6] and Bryuno [2], on the one hand the works related to formally stable systems do not consider the issue of getting estimates that measure the validity of the nonlinearly stable solutions. On the other hand the studies on elliptic equilibria from the point of view of Nekhoroshev theory have obtained very sharp bounds on the solutions but they do not deal with the existence of positive definite first integrals. The underlying idea of our criterion is connecting these worlds and getting Lie stability with the weakest possible assumptions. This is achieved by exploiting the algebraic structure of the linear part of the equation [3].

The estimates we obtain are based on a paper by Chartier *et al.* [5] where the authors determined error bounds for adiabatic invariants of Hamiltonian systems. More specifically the variation of these invariants by a truncation may remain bounded over exponentially long time intervals. Therefore, our point of view is independent of the approach of other methods mainly based in Nekhoroshev theory.

We apply our stability result to the study of the Lagrangian point  $L_4$  (or  $L_5$ ) in the spatial restricted circular three-body problem and extend previous studies [8, 1].

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## Identification of a Dynamic Metabolic Flux Model for a Mammalian Cell Culture

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The increasing demand for monoclonal antibody (mAb) has motivated the pharmaceutical industry to optimize process productivity. Monoclonal antibodies are produced through cell culture systems, in which nutrients (provided by a cell culture medium) are transformed into energy used for cell maintenance, proliferation and protein production. Because cell culture experiments and perfusion systems in particular are expensive and timeconsuming, an accurate mathematical metabolic model is a helpful tool to calculate optimal operating conditions. The current work discusses the identification of a Dynamic Metabolic Flux Model for a mammalian cell culture.

A Dynamic Metabolic Flux Model (DMFM) is a constraint-based approach where a cell is assumed to act as an optimizing agent that allocates resources to maximize/minimize a suitable biological objective. In this modeling approach, a linear programming (LP) problem solves the flux vector, at each time interval, by optimizing an objective function subject to constraints. An important advantage of dynamic metabolic flux models, as compared to other modelling approaches reported before, is that DMFM models typically require a smaller number of calibration parameters to fit/predict the data. The ultimate purpose of this research was to identify a DMFM model with a minimal number of parameters to fit and predict experimental data for batch operation of a mammalian cell culture. Two main objectives were pursued in this work: (i) - to identify a biologically meaningful objective function that mammalian cells are trying to maximize/minimize by comparing different candidates and (ii) - to systematically find a minimal set of limiting constraints. The limiting constraints were found from the values of the Lagrange multipliers of an optimization problem where the data was described by set based bounds. The developed DMFM model for CHO cells was in good agreement with data. The selected objective function involves the simultaneous maximization of growth combined with minimization of apoptosis and the limiting constraints were found to be associated to six metabolites (alanine, glutamate, lactate, ammonia, glycine, and glutamine).

## Higher Order Collocation Methods for Nonlocal Wave Equations with Inhomogeneous Boundary Conditions

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We study convergence and asymptotic compatibility of higher order collocation methods for nonlocal wave equations. The operators are inspired by peridynamics, a nonlocal formulation of continuum mechanics. The operators agree with the original peridynamic operator in the bulk of the domain and simultaneously enforce local Dirichlet or Neumann boundary conditions. We show that the methods are optimally convergent with respect to the polynomial degree of the approximation. A numerical method is said to be asymptotically compatible if the sequence of solutions  $u_{\delta}^{h}$  of the nonlocal problem converge to the solution  $u_{0}$  of the corresponding local problem as  $(\delta, h) \rightarrow (0,0)$ . We carry out a calibration process via Taylor series expansions and a scaling of the nonlocal operator via a strain energy density argument to ensure that the resulting collocation methods are asymptotically compatible. We find that, for polynomials of degree two or higher, there exists a calibration constant that is independent of  $\delta$  and h such that the resulting collocation methods for the nonlocal wave equations are asymptotically compatible. We verify this finding through extensive numerical experiments.

## Implementation, risk-analytics, and visualization of large-scale flood modeling system on Big-data framework

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#### Aim:

The traditional approach to computer simulation of flooding requires complex hydro-dynamic models which can be quite difficult to parameterize and may not lead to coherent results. In this paper we propose a method of flood inundation modeling which is robust, computationally cheap, and produces coherent, physically explainable results. Furthermore, to scale up the modeling framework for application to large watersheds, we implemented it in a big-data architecture.

#### **Study Area:**

As preliminary testing domains, we created flood inundation models for the Grand River Basin and Ottawa River Basin respectively, both located in Ontario, Canada. Each basin has experienced historical flooding and have implemented varying measures of flood control.

#### Method:

The method can broadly be divided into 3-parts: the GIS pre-processing, building regional regression model for discharge, and flood inundation model. The GIS pre-processing has been done to delineate the catchments using a digital elevation model and drainage lines provided by Environment Canada. For the stochastic discharge modeling part, first the log-spline non-parametric distribution is fitted to the yearly maximum of the station discharge values and subsequently different return period magnitudes are fitted with the corresponding upstream area using Generalized Least Square regression approach, which in-turn gives us the regional regression model for the catchments. In the last part, we use the discharge values from the regional models to inundate the catchments using catchment-integrated Manning's equation. The hydro-dynamic calculation of the inundation model has been implemented in the IBM Netezza big-data system using a Discrete Global Grid System spatial data model to scale up the model for large catchments and computing the flood inundation in real-time with user given discharge magnitudes. Furthermore, several algorithms are developed to compute risk-metrics using the stochastic flood inundation maps, which can exploit the performance of big-data and spatial data model architecture. Subsequently, a user interface was developed for user interaction with the model and output and visualization of the results.

#### **Discussion:**

The setting up of a hydro-dynamic model for any region can be complex and expensive in terms of input data and computational resources. Our stochastic flood-inundation estimation method can address the flood modeling requirements for the regions where good quality data is scarce and/or there aren't enough resources to set up a complex model. Furthermore, the model, once set up, is very fast and can be used for flood-inundation forecasting in real-time. The catchmentintegrated Manning's equation produces physically justified flood inundation extents and has a notion of volumetric conservation of water. This method, compared to the traditional solution of employing the cross-sectional Manning's equation, eliminates the need for generation of river cross-sections, which, by their design, create a high uncertainty in the flooding extent. The fast analytics powered by DGGS-big data framework allows users to quickly visualize the stochastic flood-risk and possible flood-risk for anticipated high-discharge for their region of interest. The R/Shiny framework, an open-source resource which includes spatial data handling, is dynamic and thus robust against future modifications and improvements to the proposed analytics algorithms.

## Asymptotic stability of the Novikov peakons

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#### Abstract

We prove that the peakons of the Novikov equation are asymptotically  $H^1$ -stable in the class of functions with the momentum density  $m := u - u_{xx}$  belonging to the set of non-negative finite Radon measure  $\mathcal{M}_+$ . The key ingredient in the argument is a Liouville property for the uniformly (up to translation) almost localized global solutions satisfying  $m \in \mathcal{M}_+$ , that is, we prove that such a solution must be a peakon.

## A Novel Observer based Control Scheme for Switched Impulsive Positive Systems

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This research work deals with the stability and stabilization issues on switched impulsive positive systems with time-varying delay and exogenous noise. An observer based control scheme is newly developed by considering the complex dynamic behavior. A switched impulsive positive system is described as

$$\begin{cases} \dot{x}(t) = A_{\sigma(t)}x(t) + D_{\sigma(t)}x(t - \tau(t)) + B_{\sigma(t)}u(t) + G_{\sigma(t)}\omega(t), & t \neq t_k \\ x(t) = H_{\sigma(t^-)}x(t^-), & t = t_k, \ k \in \mathbb{Z}_+ \\ y(t) = C_{\sigma(t)}x(t) \\ z(t) = C_{1,\sigma(t)}x(t) + D_{1,\sigma(t)}x(t - \tau(t)) + B_{1,\sigma(t)}u(t) + G_{1,\sigma(t)}\omega(t) \\ x(\theta) = \varphi(\theta), & \theta \in [-\tau_d, 0] \end{cases}$$
(1)

where  $x(t) \in \mathbb{R}^n_+$  is the state vector,  $u(t) \in \mathbb{R}^m$  is the control input,  $y(t) \in \mathbb{R}^y$  is the measured output,  $z(t) \in \mathbb{R}^m$  is the controlled output,  $\omega(t) \in \mathbb{R}^q$  is the disturbance input belonging to  $L_1[0, +\infty)$ .  $\tau(t)$  is the time-varying delay satisfying  $0 \le \tau(t) \le \tau$ ,  $\dot{\tau}(t) \le \tau_d$ .  $A_{\sigma(t)}, D_{\sigma(t)}, B_{\sigma(t)}, G_{\sigma(t)}, H_{\sigma(t)}, C_{1,\sigma(t)}, D_{1,\sigma(t)}, B_{1,\sigma(t)}, G_{1,\sigma(t)}$  are constant matrices with appropriate dimensions. The switching signal  $\sigma(t) : [0, +\infty) \longrightarrow \mathcal{N} = \{1, 2, \dots, N\}$  is right continuous. N is the number of subsystems,  $x(t_k^+) = x(t_k)$  and  $x(t^-) = \lim_{t \to 0^-} x(t+t)$ ;  $\{t_k\}_{k=0}^{\infty}$  with  $0 \le t_1 < \dots < t_k < \dots$ , and  $\lim_{k \to \infty} t_k = \infty$  is the switching sequence of the switching signal  $\sigma(t), t_k$  is the switching instants in which the impulsive state jump occurs simultaneously;  $t_0$  is the initial time.

This observer-based control is proposed as

$$\begin{cases} \dot{\hat{x}}(t) = A_{\sigma(t)}\hat{x}(t) + D_{\sigma(t)}\hat{x}(t - \tau(t)) + B_{\sigma(t)}u(t) + \mathfrak{L}(t), & t \neq t_k \\ \hat{x}(t) = H_{\sigma(t^-)}\hat{x}(t^-), & t = t_k, \ k \in \mathbb{Z}_+ \\ \hat{y}(t) = C_{\sigma(t)}\hat{x}(t) \end{cases}$$
(2)

$$\begin{cases} u(t) = K_{P_{\sigma(t)}}\hat{x}(t) + K_{\tau_{\sigma(t)}}\hat{x}(t - \tau(t)) \\ \mathfrak{L}(t) = L_{P_{\sigma(t)}}\left(y(t) - \hat{y}(t)\right) + L_{I_{\sigma(t-\delta_k)}}(t) \int_{t_k}^t \left(y(s) - \hat{y}(s)\right) \, \mathrm{d}s, \quad t \in [t_k, t_{k+1}) \quad k \in \mathbb{Z}_+ \end{cases}$$
(3)

where  $\hat{x}(t) \in \mathbb{R}^n_+$  is the estimated state vector,  $\hat{y}(t) \in \mathbb{R}^y$  is the observer output,  $K_{P_{\sigma(t)}}, K_{\tau_{\sigma(t)}} \in \mathbb{R}^{y \times n}$  are control gains,  $\mathfrak{L}(t)$  is the proposed observer strategy with observer gains  $L_{P_{\sigma(t)}}, L_{I_{\sigma(t-\delta_k)}}(t) \in \mathbb{R}^{n \times y}$ . This integral term gain  $L_{P_{\sigma(t)}}, L_{I_{\sigma(t-\delta_k)}}(t)$  is proposed asynchronously in terms of the time lag when switching happens. This new development is capable of improving the control performance with expected disturbance attenuation.

## A penalty-like method for CVA pricing by a PDE model

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Counterparty risk is the risk to each party of a contract that a counterparty may not live up to its contractual obligations. Counterparty risk must be evaluated properly, and the risk neutral value of a derivative must be adjusted accordingly. For the pricing of the credit valuation adjustment (CVA), or, more generally, the total valuation adjustment, known as XVA, we adopt a Black-Scholes PDE model with additional non-linear terms [3]. We formulate Dirichlet boundary conditions using the techniques in [1, 2]. For the discretization, we use standard second order differences in space and Crank-Nicolson timestepping. For the treatment of the nonlinearity, we formulate a penalty-like iteration motivated by [4]. We present numerical experiments indicating that the penalty method converges in about one iteration per timestep, irrespectively of the discretization size, and that second order convergence is exhibited.

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## **Adaptive Radial Basis Functions for Embedded Surfaces**

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We present a numerical method for solving reaction-diffusion systems and other PDE problems on curved surfaces and other general domains. Our method is similar to the work of Petras, Ling, Piret, and Ruuth [1, 2] in that it combines the closest point method [3] with radial basis function finite differences for derivatives and interpolation.

Closest point methods work by embedding the original surface problem in a higher-dimensional space. We leverage the penalty approach of [4] to constrain the solution in the embedding space to be constant in the normal direction off of the surface. This approach has been shown to work well with finite difference methods and enables both implicit and explicit time-stepping.

The computational domain is a narrow band of points enveloping the surface. These points can be scattered or sampled from a uniform grid. We experiment with local adaptivity, either refining the grid locally or clustering points near regions of high surface curvature and/or regions with fine-scale solution features. We show some preliminary results of non-uniform pattern formation on curved surfaces.

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## About the Algorithms of Strategic Management

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This article is devoted to development of generalized dynamical programming methods of mathematical and computational approaches for solving optimization problems in modern business. Investigation is focused on discrete dynamic modeling of project management in corporate network of company [1]. Graph theory applications to build of planning approach of project selection are discussed [2]. The tools applied in this work based on the priority queue implementation allow the development of algorithms effective management strategies.

There are the following sub-problems discussed:

- Investigation dynamic model of multistage plan of project selection in corporate network company
- Investigation method of generalized dynamical programming approaches
- Justify an algorithms of solution
- Create a pseudo code for software implementation.

The results will be presented on both the fundamental and applied level

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## **Gauge Theory and Boundary Conditions in Spin Ice Thin Films**

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Spin Ices are classic examples of frustrated magnets, magnetic materials which do not exhibit an ordering transition down to the lowest temperatures due to energetically competing interactions and crystalline geometric constraints which lead to a highly degenerate ground state. Consequently, these materials exhibit a highly correlated yet disordered low-temperature phase referred to as a spin liquid. In the simplest classical cases, the system can be described by a divergenceless vector field representing the orientations of the spins, reminiscent of the magnetic field of electromagnetism [1]. The low energy excitations can then be interpreted as playing the role of magnetic monopoles which are created and destroyed in pairs. The analogy can be taken even further when considering the quantum theory of spin ices, in which a U(1) gauge theory emerges with both magnetic and electric charges and emergent photons directly analogous to Quantum Electrodynamics [2].

Such spin liquid phases described by an emergent gauge field are not uncommon, but to date, no theory has been constructed to explain the role of boundary conditions on the physics of such systems. Boundary conditions play an important role in classical electromagnetism, and developing an understanding of their role in spin ice is necessary to complete its "magneto-electric" description. More importantly, having a theory of boundary conditions will be necessary for the potential development of "magnetronic" technologies and other applications such as spin ice heterostructures, as well as for understanding the physics of extended defects in spin ice crystals. Recently, experiments have begun to explore the effects of boundaries by studying thin films of spin ice compounds just a few nanometers thick [3, 4, 5], making the development of such a theory all the more pressing. In this talk, I will discuss the current status of the construction of a classical mathematical model of spin ice thin films and the understanding of the role of boundary conditions in modifying the near-surface properties of these materials. This is currently being done through the use of both a large-*N*, or spherical, model which can be solved exactly, exhibiting interesting new behavior such as oscillations in correlation strengths near the film edge, as well as a coarse-grained theory of magnetic fluxes described by a divergenceless vector field in the bulk, whose behavior is non-trivially modified by the geometry of the exposed film surface.

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## **Spontaneous Symmetry-Breaking in Deterministic Queueing Models with Delayed Information**

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In queueing theory, a fluid model is a mathematical model which describes the fluid level in a reservoir where the periods of filling and emptying are randomly determined. Recently, a deterministic fluid model was constructed and analyzed in [4, 5] to describe the dynamical behavior of a system involving two queues. Their model incorporates customer choice behavior based on delayed queue length information. That is, the information given to the customers is based on the queue length information from a previous time and not on the current time. Waiting times in emergency rooms of hospitals, telephone call centers, and various rides in theme parks are some examples where in delayed information are provided to the customers. This time delay has an impact on the dynamical behavior of the queues and therefore has the capacity to affect the decision of a customer to choose which queue to wait in.

We generalize the queueing model studied in [4, 5] into *N* number of queues. The system of delay differential equations for this generalized model is equivariant under the finite symmetric group  $S_N$ . Spontaneous symmetrybreaking occurs in an equivariant dynamical system when the symmetry group of a solution of the equations is lesser than the symmetry group of the equations themselves [3]. In this work, we use group-theoretic techniques [1, 2] to show that the generalized model exhibits spontaneous symmetry-breaking. This, in turn, allows us to determine which type of solutions that can only occur in the system. In particular, we show that varying the time delay parameter can make a stable fully-symmetric equilibrium becomes unstable. This switch in stability occurs only at a symmetry-breaking Hopf bifurcation, that is, the branch of periodic solutions that bifurcates has lesser symmetry than the branch of fully-symmetric equilibria. Understanding such dynamical behavior of queues caused by providing delayed information to the customers provides insights that are beneficial for managers and operators of queueing systems.

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## A Parallel Implementation of the Delay Stochastic Simulation Algorithm

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Biochemical reaction systems are commonly studied by numerically simulating their trajectories over time using Monte Carlo approaches, such as the popular Stochastic Simulation Algorithm (SSA) that takes into account randomness that may occur. For some complex models such as tumor growth, an additional element called delay comes into play and makes the biochemical reaction systems more intricate because it becomes necessary to account for the time it takes to complete certain reactions. Here we consider the Delay SSA to simulate such models. A prevalent setback of the SSA is computational time, which gets even longer when we incorporate delay. We describe how our work speeds up the calculations using parallel processing.

The SSA by Gillespie [1] examines the time evolution of a chemical reaction system using a discrete stochastic process using random numbers to draw sample paths of the state vector  $\mathbf{X}(t)$  over time. Each reaction has a propensity function  $\alpha_j$ , which captures how likely that one reaction will occur in  $[t, t + \tau)$ . The Delay Stochastic Simulation Algorithm (DSSA) is a variant that takes into account the fact that some reactions may complete after a delay instead of instantaneously as assumed by the classic SSA. We denote the delay constant as  $\sigma \ge 0$  and  $\sigma \in \mathbb{R}$  [3].

In [5], Barrio et al. adapt the SSA in order to capture delay associated with systems that involve waiting periods between the times that reactions start and finish. In [3, 4], Barbuti et al. adapt the SSA in order to capture delay as a waiting period and as the time needed to prepare a reaction for execution while other reactions continue to execute. We examine delay that occurs naturally in the application of the cell cycle of tumor cells [2]. The cell cycle describes the events of the process of cell replication and cell division (mitosis).

Our results show that the DSSA can be implemented in parallel to decrease the computational time of simulating biochemical reaction systems. The process is useful for larger systems with many more species and reactions because the computational time will be longer. The numerical results show that by implementing parallel processing the computational time is decreased and the efficiency is improved.

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## On co-orbital quasi-periodic motion of two small moons around a large planet

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Celestial Mechanics refers to co-orbital motion when two or more bodies, such as planets, moons or asteroids, orbiting at the same, or very similar, distance from their central body, that is, are in a 1:1 mean-motion resonance. There are several types of co-orbital objects, depending on their point of libration. One class is the horseshoe orbit, in which objects librate around 180° from the central body. A small number of asteroids has been found that are co-orbital with Earth, like asteroid 3753 Cruithne. But, among all examples, since their discovery in 1981 by the spacecraft Voyager 1, the Saturnian moons, Janus and Epimetheus, is one of the most known co-orbital horseshoe orbit.

When the co-orbital motion is considered one has to keep in mind that the distance between the orbits of the small bodies is also small and their interaction will become large when the two small bodies are close. Due to it, there are three small quantities to consider. Following the ideas in [1], we assume that the difference between the semi-major axes of the orbits when the small bodies are far apart is of order  $\varepsilon$  compared with the average radius of their orbits. Second, we assume that the masses of the small bodies are of order  $\varepsilon^a$  compared to the big mass or central body. Finally, since we are looking for orbits that have no syzygy when the small bodies are in the same side of the central body, we asume that the minimum angular separation, if we look at the particles from the big mass, is of order  $\varepsilon^b$ .

Then, within the framework of the planar three-body problem we establish the existence of quasi-periodic motions and KAM 4-tori related to the co-orbital motion of two small moons about a large planet where the moons move in nearly circular orbits with almost equal radii. The approach is based on a combination of normal form and symplectic reduction theories and the application of a KAM theorem for high-order degenerate systems. To accomplish our results we need to expand the Hamiltonian of the three-body problem as a perturbation of two uncoupled Kepler problems. This approximation is valid in the region of phase space where co-orbital solutions occur [2]. As far as we know there are not similar studies dealing with the persistence of invariant 4-tori for the co-orbital motion of the three-body problem.

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## Algebraic Structure of the Varikon Box

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The 15-Puzzle is a well studied permutation puzzle. This work explores the group structure of a threedimensional variant of the 15-Puzzle known as the Varikon Box, with the goal of providing a heuristic or algorithm for solving it while minimizing the number of moves. First, we prove by a parity argument which configurations of the puzzle are reachable. We define a generating set based on the three dimensions of movement, which generates a group that acts on the puzzle configurations, and we explore the structure of this group. Finally, we show a solution can be given by writing an element of the symmetric group as a word in terms of a generating set, and we compute the shortest possible word for each configuration.

## **Time-parallelization of hyperbolic equations with MGRIT**

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In order to accelerate the numerical solution of evolving PDEs and ODEs, a variety of time-parallelization methods have been proposed over the last few decades [1]. These techniques seek parallelization by splitting among different processors the computation of the solution along the time domain, thus providing an additional direction for parallelization when classical spatial domain decomposition schemes saturate. Among parallel-in-time methods, the *Multigrid Reduction In Time* (MGRIT, [2]) algorithm, which can be interpreted as a multigrid scheme with the coarsening procedure acting along the time domain, is one of the most developed and studied in the literature.

While time-parallelization has proven to be very effective when used to speed up the solution of parabolic equations, its applicability to advection-dominated or hyperbolic PDEs still remains a matter of research. Growth of instabilities and slow convergence are both strong issues in this case, which end up neglecting most of the advantages from parallelization, even though some successfull examples have been reported (*e.g.*, in [3, 4]).

In our work, we investigate in detail the performance of MGRIT when applied to non-linear hyperbolic problems, testing it on a variety of discretization schemes. Our study focuses on determining the principal factors that cause degradation in the convergence speed of the algorithm, and identifies some future directions for improvements.

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## The Effects of Dielectric Decrement and Finite Ion Size on Differential Capacitance of Electrolytically Gated Graphene

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Since its discovery, graphene has found numerous applications in electronics and photonics. Due to its unique properties, graphene has risen to be one of the key materials of interest in the development of nanoscale biological and chemical sensors [1, 2, 3]. Graphene-based sensors show great promise in their ability to accurately detect changes to their environment, such as specific concentrations of molecules of interest or to acidity [4, 5].

While there has been plenty of experimental research conducted in regards to the viability and sensitivity of graphene-based devices, there has been a significant lag in the scientific theory to understand the microscopic and macroscopic physics of these sensors, which is unlike any other areas of applications for graphene [1, 2]. While there has been some success in modelling these sensors [6, 7, 8], there is still very little theoretical work to account for the vast extent of experimental work. Without a full theoretical understanding of the background for the role graphene plays in these sensors, the development and implementation of these devices is plagued.

In this work, we analyze the effects of dielectric decrement and finite ion size in an aqueous electrolyte on the capacitance of a graphene electrode, and make comparisons with the effects of dielectric saturation combined with finite ion size. We derive conditions for the cross-over from a camel-shaped to a bell-shaped capacitance of the diffuse layer and show that the total capacitance is dominated by a V-shaped quantum capacitance of graphene at low potentials. A broad peak develops in the total capacitance at high potentials, which is sensitive to the ion size with dielectric saturation, but is stable with dielectric decrement.

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#### Thermal and Pollution Aspects of a Storage Water Heater Affected by Flue Baffles

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In this paper, the main goal is to understand how effective the flue baffles are in a storage water heater regarding the thermos-chemical properties of the flue gases (exhaust gases). To do this, we first assess our numerical analysis [1-4] solving a kerosene-fired burner (configuration 1) and examining the differences which might exist between our numerical results and the data of experiment [5]. The contrast reveals that our numerical analysis would be accurate for the prediction of thermos-chemical properties of the flame. Then, we change the geometrical configuration of the combustor equipping it to a flue tube (chimney) for collecting the flue gases and delivering to the outside atmosphere (configuration 2). To mimic the thermal behavior of the storage water heater, we consider suitable boundary conditions for the flue tube. We simulate this new configuration numerically and present the contours of temperature and soot concentration inside the computational domain. Afterwards, we equip the flue tube of the configuration 2 to few flue baffles, mounted inside the chimney (configuration 3). Similarly, we simulate the new configuration numerically and, again, present the contours of quantities inside the computational domain. We compare together the correspondent contours obtained for the burners 2 (without any flue baffles) and 3 (with flue baffles) to clearly present the differences between them. Such comparison can clarify the effects of the flue baffles on the thermos-chemical properties of the exhaust gases. To the best of our knowledge, there is not a study in the literature discussing these effects. Our findings indicate that flue baffles are influential in changing the thermos-chemical aspects of the storage water heater. They show that the flue baffles improve the heat transfer through the flue tube. They increase the soot concentration in the exhaust gases discharging into the outside atmosphere. This study is fully completed by now. In other words, the full paper is ready to be submitted to AMMCS2019 by request (upon the acceptance of this one-page abstract). The current study provides a deep insight for the researchers and helps the designers to improve the designs of new storage water heaters.

Keywords: Combustion; Pollution; Combustor; Storage Water Heater; Flue Baffles

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## **Elliptic Curves of Prime Conductor**

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The torsion order elliptic curves over the rationals, Q, with prime conductor have been well studied. In particular, we know that for an elliptic curve E/Q with conductor p a prime, if p > 37, then E has either no torsion, or is a Neumann-Setzer curve and has torsion order 2. In this talk we examine similar behavior for elliptic curves of prime conductor defined over totally real number fields.

## Sensitivity relationships for optimal control problems with endpoint constraints. Applications to trajectory optimization of space launchers.

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In this talk we will present a new numerical approach to solve optimal control problems of Mayer type with endpoint constraints. The key issue of the proposed method is to use the link between a value function associated with the optimal control problem and the optimality conditions coming from the Pontryagin's maximum principle (PMP). Many authors ([1, 2, 3]) mention that in the case of endpoint constrained problems such relations are much more difficult to define. In particular because the value function in such case is in general l.s.c. In the approach presented in this talk, we define an auxiliary augmented value function that is Lipschitz continuous and allows to establish the sensitivity relations. This value function can be computed as a solution of a Hamilton-Jacobi type equation. Using the sensitivity relations we can estimate an approximation of the optimal adjoint state at the initial time from this auxiliary value function. Then the system of optimality conditions from the Pontryagin's principle can be integrated to compute the optimal trajectory.

These new theoretical results was applied recently to a real industrial problem in the domain of the trajectory optimization for heavy space launchers. We will present in this talk an example of numerical results obtained for a trajectory optimization problem for a two-stage heavy launch vehicle.

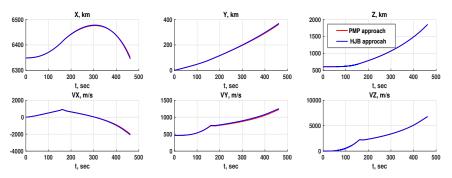


Figure 1: Example of optimal trajectory: in red, the trajectory computed by CNES with a shooting method (PMP) and in blue : the trajectory obtained using HJB approach linked with PMP.

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## **Machine Learning Techniques for Insurance Applications**

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Predictive analytics is gaining increased importance in the insurance industry. Applications of machine learning techniques cast light in the insurance problems and boost performance when calculating insurance quantities. In this talk, we will give two examples. Our first work applies machine learning techniques to credibility theory, a cornerstone of actuarial science, and proposes a regression-tree-based algorithm to integrate covariate information into credibility premium prediction. The recursive binary algorithm partitions a collective of individual risks into mutually exclusive sub-collectives, and applies the classical Buhlmann-Straub[1] credibility formula for the prediction of individual net premiums. The algorithm provides a flexible way to integrate covariate information into individual net premiums prediction. It is appealing for capturing non-linear and/or interaction covariate effects. It automatically selects influential covariate variables for premium prediction and requires no additional ex-ante variable selection procedure. Last but not least, it is superior in prediction accuracy. Our second work is in the context of mortality forecasting, which is fundamental to life insurance pricing. The Lee-Carter[2] model has been the benchmark mortality forecasting method and the Li-Lee[3] approach extends it by taking into account the similar patterns from a group of populations. We further improve the Li-Lee approach by designing a DSA (deletion/substitution/addition) iterative algorithm to dynamically select a group of countries in a data-driven manner. Our work provides a guide on a group of countries sharing similar mortality patterns for each individual country and improves mortality forecasting accuracy greatly.

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## Self-Similarity in the Kepler-Heisenberg Problem

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The Kepler-Heisenberg problem is that of determining the motion of a planet around a sun in the Heisenberg group, thought of as a three-dimensional sub-Riemannian manifold. The sub-Riemannian Hamiltonian provides the kinetic energy, and the gravitational potential is given by the fundamental solution to the sub-Laplacian. The dynamics are at least partially integrable, possessing two first integrals as well as a dilational momentum which is conserved by orbits with zero energy (see [?]). The system is known to admit closed orbits of any rational rotation number, which all lie within the fundamental zero energy integrable subsystem (see [?, ?]). Here, we demonstrate that all zero energy orbits are self-similar.

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## Mathematical Model of a Brain-on-a-Chip for Studying the Role of the Nitric Oxide Dynamics in Cerebral Microaneurysms

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Cerebral microaneurysms are abnormal swellings of small blood vessels in the brain with high risk of rupture. They can form on arterioles located either in the retinas of diabetic patients, of deeper inside the brain tissue. Ruptures of microaneurysms could cause life-threatening intracranial hemorrhages, or, in the case of diabetic retinopathy, could lead to blindness. Except for retinal microaneurysms, localizing microaneurysms before they rupture is very hard because there may be no symptoms, or the symptoms can be easily accredited to other more common brain disorders. Mathematical models can provide useful insights into mechanisms of aneurysmal development and suggest specialized biomarkers for aneurysms. Most of the mathematical models of intracranial aneurysms describe mechanical interactions between blood flow and arteries. However, these models do not work for microaneurysms because the anatomy and physiology at the length scale of cerebral microcirculation are different from those of the macroscopic circulation. Some recent progress on the modeling of cerebral microaneurysms were reported in [1, 2].

In [3], I introduced the concept of a brain-on-a-chip and proposed a mathematical framework for studies of mechano-electrochemistry of brain. A brain-on-a-chip is an engineered neuro-glial-vascular unit optimized to perform certain fundamental functions. Here I present a mathematical model of a brain-on-a-chip specialized to study the possible role of the nitric oxide dynamics in the development of cerebral microaneurysms. The proposed brain-on-a-chip is made of a neuron modeled as a linear viscoelastic Kelvin-Voigt solid whose ionic gates are linear viscoelastic Maxwell fluids, and an astrocyte represented either by one endfoot controlling vasodilatation or two endfeet regulating opposite vasomotor responses. The endfoot modulating vasodilatation is a spring-mass system coupled to the viscoelastic and mass elements representing the neuron and its membrane. Two forces proportional to the concentration of nitric oxide act on the neuron and the endfoot regulating vasodilatation. These rheological elements are further coupled with the Hodgkin-Huxley electrical circuit. A Lagrangian formulation and a non-conservative Hamilton's principle are used to obtain the corresponding Euler-Lagrange equations. The effects of the nitric oxide produced by neurons and endothelial cells on the mechano-electrochemical behavior of the proposed brain-on-a-chip are investigated through numerical simulations. Our results suggest that a non-decaying synthesis of nitric oxide may be a contributing factor in the formation and growth of a microaneurysm. This suggests that the onset of microaneurysms could be caused by a combination of deviant mechanical pushing of the vascular wall by the blood flow and anomalous chemicallyinduced pulling of the wall exerted by the neuro-glial-vascular unit. More details on this model are given in [2].

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## Functional and thermodynamic limits of a simple stylized model for the distribution of wealth

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We consider a simple finitary random exchange model [1] with n "coins" shared within N "agents"; the model is represented by a Markov chain with transition probability given by

$$\mathbf{P}\{\mathbf{Y}(t+1) = \mathbf{n}' | \mathbf{Y}(t) = \mathbf{n}\} = \sum_{i,j:i \neq j} \left\{ \frac{1}{N} \frac{1}{N-1} \left( \frac{11\{n_i + n_j \ge 1, n'_j \ge 1\}}{n_i + n_j} + 11\{n_i + n_j = 0\} \right) \delta_{n_i + n_j, n'_i + n'_j} \prod_{k \neq i,j} \delta_{n'_k, n_k} \right\},$$

where  $\mathbf{Y}(t)$  denotes the state of the system at step t living on the scaled integer symplex

$$S_{N-1}^{(n)} = n\Delta_{N-1} \cap \mathbf{Z}^{N} = \left\{ \mathbf{n} = (n_{1}, n_{2}, \dots, n_{N}) : 0 \le n_{i} \le n, \quad \sum_{i=1}^{N} n_{i} = n, \quad n_{i} \in \mathbf{N}_{0}. \right\}.$$

As a functional limit, we derive a discrete-time continuous state space Markov chain and we study its stability. If  $W_N$  denotes total wealth with N agents and  $X_i = W_i/W_N$  the fraction of wealth of each agent, the invariant and equilibrium distribution of the latter chain is the uniform distribution on the simplex

$$\Delta_{N-1} = \left\{ \mathbf{x} = (x_1, \dots, x_N) : x_i \ge 0 \ \forall i \in 1, \dots, N, \quad \sum_{i=1}^N x_i = 1 \right\}.$$

Therefore, thanks to exchangeability, we are able to derive the wealth distribution as the marginal of the uniform distribution on a single agent. We then consider the thermodynamic limit  $N \to \infty$  both when  $W_N/N \to w < \infty$  (linear growth of wealth) and when  $W_N/N \to 0$ . Using the Poissonization trick due to Kac and martingale methods, we are able to derive Boltzmann kinetic equations for the wealth distribution  $\mu_t$  in weak form

$$\mu_t = \mu_0 + \int_0^t Q(\mu_s) \ ds,$$

where the operator Q is defined as follows: for any  $g \in C_b(\mathbf{R}_+)$ 

$$\langle g, Q(\mu) \rangle = \int_{[0,1]} dr \int_{\mathbf{R}^2_+} \mu(dx) \mu(dy) \left( g(r(x+y)) + g((1-r)(x+y)) - g(x) - g(y) \right) 1\!\!1_{\{x+y \le w_0\}},$$

with  $w_0 = \lim_{N\to\infty} W_N$ . In the large time limit  $t \to \infty$ , the solutions to kinetic equations do coincide with the corresponding limits of the marginals of the Markov chain. In summary, in this simple case, we are able to complete Boltzmann's program starting from a "microscopic" discrete (finitary) model and leading to kinetic equations in the thermodynamic limit thanks to the presence of symmetries (exchangeability). By beginning with a discrete microscopic model described by a Markov chain, we do not need *ad hoc* hypotheses such as the *Stoßzahlansatz*.

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## **Coupling Decomposition with Dynamic Programming : An Overview Applied to an Energy Management Model**

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The problem we will tackle in this talk is a continuous differentiable linear stochastic model. The problem we want to solve in its simple form can be written :

$$\min_{p,f,u,x} E_{\mathbf{d},\mathbf{i}} \left[ \sum_{\tau=1}^{T} \left( \sum_{z \in Z} c_{z\tau} p_{z\tau} + l_{\tau} f_{\tau} \right) + \sum_{z \in Z} F_z(x_{zT}) \right]$$
(1)

s.t. 
$$u_{z\tau} + p_{z\tau} - Af_{\tau} = \mathbf{d}_{z\tau}, \quad \forall z \in \mathbb{Z}, \tau \in [1, T]$$
 (2)

$$x_{z,\tau} = x_{z,\tau-1} - u_{z\tau} + \mathbf{i}_{z\tau}, \quad \forall z \in \mathbb{Z}, \tau \in [1,T]$$
(3)

with bounds on all variables and bold variables considered stochastic. A part of the difficulty in solving this model comes from the stochasticity of the problem : each  $\mathbf{d}_{z,t}$  and  $\mathbf{i}_{z,t}$  is a stochastic process. Even if we were to discretize each of them in various scenarios (say *N* at each time step), then we get  $N^T$  different scenarios for each process, making direct solving of this problem intractable as *T* gets large [1] (even for N = 2 or 3 since we take *T* typically in the hundreds). This talk focuses on the fact that this problem has multiple couplings, in fact there are :

a coupling on indexes z through constraints (2) (coupling in space);

a coupling on indexes t through constraints (3) (coupling in time);

a coupling on the stochasticity of the scenarios through the nonanticipativity contraints.

Although this problem can get large, it has an interesting structure which we can use to ease its solution. This presentation aims at pointing out different aspects and interpretations of decoupling for this kind of problem. Decomposition of this model in zonal subproblems seems an appropriate way to go since we know effective ways to solve such subproblems, such as SDDP [2]. An instance of this problem (which is an hydroenergy management problem) was solved using multiple methods, including a direct solve of the problem and decomposition through ADMM and Dynamic Programming (see [3] for a survey on decomposition methods). The methods were implemented in Julia 1.1, mainly using IPOPT to solve subproblems arising in our decomposition schemes as well as to find a direct solution for small instances.

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## Positron Emission Tomography Image Resolution Limit when using the Likelihood Model with Excellent Time-of-Flight Resolution

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Positron Emission Tomography (PET) is a medical imaging modality that enables the observation of metabolic processes by creating an image of a radiotracer distribution in a subject. The data acquisition consists of detecting the arrival times and positions of the annihilation photon pairs emitted by the radiotracer. Since each pairs travel path is mostly collinear, their origin can be evaluated in theory. However, the current resolution of annihilation photon timing, called Time-of-Flight (ToF), induces a blur of at least one centimeter which is impracticable for medical imaging. Optimization models, the most used being the likelihood, circumvent that limitation. Recent developments in ToF resolution indicate that analytical image formation, without loss of resolution, could be available in the future. We are interested in evaluating if optimization models, with their capacity to incorporate complex *a priori* information, remains pertinent in PET imaging even when excellent ToF resolution is available.

This investigation focus on the image resolution limit in that context. Previously, it was established that this limit was determined by the combination of data sampling constraints and physics-induced blur [1]. We demonstrated that the detector size could be mitigated when excellent ToF resolution was used in the likelihood model [2]. When we further investigated the resolution limit by using Monte Carlo simulations and neglecting physics-induced blurs in the reconstruction model, we have observed that resolution better than the one defined by the physics-induced blurs could be obtained and that, in some cases, the reconstructed signal position was biased. These observations goes against the intuition that an image reconstructed with the PET likelihood model, in which physics-induced blur is neglected, is the true radiotracer distribution blurred by the response functions of the physical phenomenons. This intuition is due to the fact that PET acquisition can be modeled as a Radon transform for which the resolution is demonstrated to be lower-bounded by these physical factors. The inclusion of physics-induced blur in the reconstruction model requires substantial computation ressources.

The investigation that we present in this talk will be divided in two parts. Firstly, we will compare the resolution property of the image obtained using the likelihood model to the one obtained using the inverse Radon transform when physics-induced blur is neglected in both reconstruction process. It is paramount to understand the impact of neglecting these phenomena on the likelihood model since our previous investigation indicates that it differs from the analytical approach. Secondly, we will compare optimal solution of the the ToF likelihood model with the one of the ToF-less likelihood model. The inclusion of ToF information in the PET reconstruction process, in short, introduces a new dimension to the data sampling space and is straightforward to deduce from its ToF-less counterpart. The bias in signal position observed previously indicates that the PET ToF likelihood model might not be suitable for high ToF resolution. To investigate the potential of optimization models combined with high ToF resolution, we first investigate the limit of the PET ToF likelihood model.

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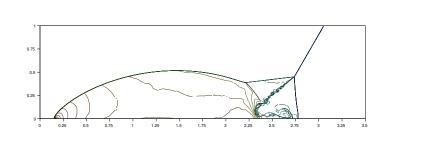
## Limiting on adaptively refined, nonconforming meshes

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Numerical solutions of hyperbolic conservation laws using higher order methods like the discontinuous Galerkin (DG) method often develop spurious oscillations, which may lead to instabilities in the solution. Limiting is one of the mechanisms used to suppress such oscillations. DG specific limiters like Barth-Jesperson and moment limiters were proposed in Refs. [1, 2] for conformal meshes, which require the numerical solution in the neighbourhood of an element. In this work, we extend these limiters to nonconforming meshes which arise in adaptive computations. Compared to an element in a conformal mesh, an element in a nonconforming mesh can have a higher number of elements in its neighbourhood, where the neighbouring elements may be of different sizes. Further, the neighbourhood of an element may change with every adaptive refinement of the mesh. We propose a novel algorithm to update the neighbourhood of elements in an adaptively refined mesh on a graphics processing unit, by maintaining a database of the vertices in the mesh and the elements associated with each of the vertex. Our algorithm is implemented entirely on the GPU and avoids race conditions. We provide numerical experiments to validate the robustness and accuracy of the algorithm. For example, Fig. 1 shows the density isolines at t = 0.2 for the double Mach test case, obtained with the moment limiter over Barth-Jesperson limiter with respect to the computational cost involved in setting up the neighbourhood and executing the limiters.



(a) Density isolines.

(b) Zoom on slip line region.

Figure 1: Density isolines at t = 0.2 for double Mach test case.

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### SuperNet: Using Supermodeling in Developing More Efficient Data Models

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Supermodeling is a new approach for modeling complex dynamical systems where the Supermodel is composed of a few dynamically coupled *sub-models*. As shown in (e.g., Ref.[1]), it can distinctly outperform of the best sub-model in prediction accuracy. This modeling strategy can be extended on complex data models such as deep neural networks (DNNs), particularly, convolutional neural networks (CNNs). While a single DNN can be treated on its own as the classical ensemble classifier, the SuperNet represents the next abstraction level. In the former, DNN consists of plethora tightly coupled unstable weak classifiers (neurons) while in the latter, the SuperNet integrates only a few and weakly connected strong classifiers (DNNs). The novelty of our approach, over traditional ensembling methods and Stacked Neuron Networks (S-NN) Ref. [2], is in coupling of a few pretrained DNNs via the last output layer. Only this layer of the SuperNet is additionally trained (see Fig.1a). As shown by example result from Fig.1b, this type of dynamic ensembling can outperform the accuracy of both the best results obtained by the sub-nets and other typical ensembling method (such as bagging, majority and k-Borda voting). Because the sub-nets can represent various sub-optima instances obtained during training of a single DNN which can be sampled by using fast algorithms proposed in Ref.[2,3], and for the SuperNet only the output layer needs to be learned (only a few epochs are needed, see Fig.1b green line), the computational time overhead caused by the SuperNet is insignificant comparing to the learning time of a single DNN. We discuss also preliminary results of SuperNet accuracy in Transfer Learning Ref.[1], which demonstrate that a few sub-nets, pretrained for various types of datasets of images, can create very general and robust SuperNet. It can be used for classification of a new category of images, which size (e.g., small number of samples, high dimensionality) is insufficient to train a unique CNN. We show that also in this case the SuperNet can produce meaningful classification results.

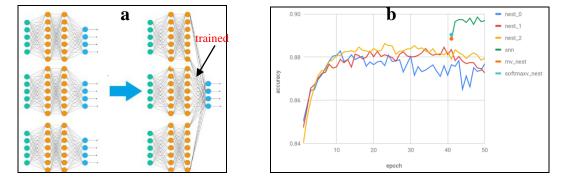


Figure 1: The SuperNet (a) and example result of its accuracy (*snn*, green line) (b) after trained sub-nets integration. The plot shows the results for all DNNs sub-nets with training epoch on the "fashion" MNIST (FMNIST) dataset (training:  $6 \cdot 10^4$  and test:  $10^4$  images). The accuracies were obtained on the test data. The orange and green dots show the accuracies for majority voting (*mv\_nest*) and bagging (*softmax\_nest*) ensembling methods, respectively.

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## **Disease Dynamics Inferred from Last Wills and Testaments**

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Historical epidemics of infectious diseases are often studied through mortality records. In England, registration of deaths began in 1538, long after the invasion of the Black Death in the 14th century. Some historical research on the Black Death has been based on monthly counts of wills written in London during known plague epidemics. We undertook a systematic analysis of all wills probated in the Court of Husting, London, 1258-1688.

These wills were digitized in 2017 by British History Online. We wrote an R package that scrapes the wills from the web and provides tools to perform a variety of statistical analyses. We aimed to contribute both to historical epidemiology and to other historical work on Medieval and Renaissance London.

There were 4,110 wills probated by Court of Husting. The date of probate is known for all wills, but the date the will was written is indicated in only 64%. Only 11% of testators were women. Of the 51% of wills that mention an occupation, 82% were merchants, and all others were members of the church, municipal government, or nobility. We obtained a daily time series of numbers of wills written, and a weekly time series of numbers of wills probated (because wills were probated only on Mondays). Four large peaks (during known plague epidemics in 1348, 1361, 1368 and 1375) are clear. Plausible epidemic growth rates can be estimated using will dates, but not probate dates. The distribution of lags from writing to probating wills is approximately lognormal.

## **Triskelion Structured Small Colloidal Semiconductor Quantum Dots**

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We show, using density functional theory and ab initio molecular dynamics, that certain small colloidal semiconductor quantum dots with a mixed nanocrystal core that is capped with achiral surface ligands spontaneously form a triskelion structure (with  $C_3$  symmetry) which is persistent at room temperature when capped amine ligands. Furthermore, the nanocrystal core also adopts the triskelion structure. The focus of our study is a colloidal quantum dot with a  $Cd_{16}Se_7Te_3$  core (and a charge of +12) capped with negatively charged surface ligands to achieve charge neutrality- in the simplest instance, twelve Cl<sup>-</sup> ligands to form the colloidal quantum dot  $Cd_{16}Se_7Te_3Cl_{12}$ . The small size of the core (for which almost all atoms are surface atoms), the high positive charge that destabilizes the core, the mixed (Cd/Te) composition that creates mechanical strain in the core, and the inclusion of precisely three Te atoms in the predominantly Se core, all play critical roles in the spontaneous formation of the triskelion structure.

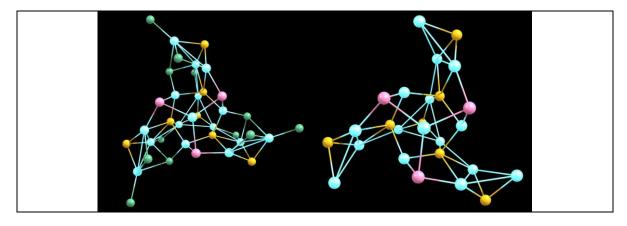


Figure 1: Optimized Structure of Triskelion Colloidal Quantum Dot

## A Bestiary of Transformation Semigroups for the Holonomy Decomposition

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The Krohn-Rhodes theorem decomposes a finite discrete dynamical system hierarchically into simpler components, namely as a cascade of levels of parallel flip-flops and permutation groups augmented by reset maps [1]. Computationally tractable implementations of this mathematical theorem are now available in computer algebra systems [2, 3]. These rely on the holonomy decomposition method of proving the Krohn-Rhodes theorem [4, 5, 6, 7, 8], which studies the structure and covering relationships of image sets and their permutators.

The development of the computational implementation of the holonomy decomposition was not a straightforward process. This is often the case with any software project, and the open mathematical questions about the algorithm added more difficulty. The computational exploration, the testing and debugging cycles produced an interesting set of example transformation semigroups. These include illustrative examples, and examples that cover 'edge cases' and exhibit unexpected features possible in discrete dynamical systems. Here, we will analyse these semigroups in order to shed light on the inner workings of the decomposition algorithm. In particular, we will demonstrate the possibility of

- non-image tiles, i.e. maximal subsets covering a state set *P* that cannot be accessed through the dynamics of the semigroup from *P*;
- transformation semigroups with very wide or very tall skeletons;
- sets appearing lower in the hierarchy than sets with fewer elements;
- non-isomorphic permutator and holonomy groups of the same set of states; and
- overlapping tiling covers for non-equivalent sets.

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## Iron Doped Gold Cluster Nanomagnets: *Ab Initio* Determination of Barriers for Demagnetization

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Magnetic properties of small- and nano-sized iron doped gold clusters are calculated at the level of second order multireference perturbation theory. We first assess the methodology for small Au<sub>6</sub>Fe and Au<sub>7</sub>Fe clusters, which are representative of even and odd electron count systems. We find that larger active spaces are needed for the odd electron count system, Au<sub>7</sub>Fe, which exhibits isotropic magnetization behaviour. On the other hand, the even electron count system, Au<sub>6</sub>Fe, exhibits strong axial magnetic anisotropy. We then apply this methodology to the tetrahedral and truncated pyramidal nano-sized Au<sub>19</sub>Fe (with S=3/2) and Au<sub>18</sub>Fe (with S=2) clusters. We find that face substitutions result in the most stable structures, followed by edge and corner substitutions. However, for Au<sub>18</sub>Fe, corner substitution results in strong magnetic anisotropy and a large barrier for demagnetization while face substituted Au<sub>18</sub>Fe can act as a single nanoparticle magnet [1].

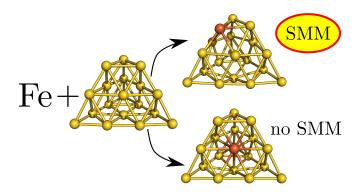


Figure 1: Single molecule magnet properties depend on the substitution scheme.

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# **Engineering Quantum Defects in Polycrystalline Diamonds for Magnetic Field Sensing Application**

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Impurities like nitrogen trapped by defects in diamonds can function as an electronic solid-state spin sensor with potential applications in quantum computing and magnetic field sensing [1]. The incorporation of nitrogen impurities into diamonds can lead to the formation of nitrogen-vacancy (NV) optical centers with long spin coherence time. The long spin coherence time of NV centers at ambient temperatures and an efficient means of manipulation/optical read-out has necessitated its inclusion in the list of highly sensitive detectors. In recent years, there has been an effort towards the development of low-field magnetic resonance imagers (MRI) due to their low cost and accessibility [2]. Despite the progress, low-field MRIs suffers from low signal-to-noise (SNR) when compared to their high-field counterparts.

To improve the SNR of low-field MRIs, we are currently developing quantum sensors to collect nuclear magnetic resonance (NMR) signals with better sensitivity. In this study, quantum defects in diamond located at about 200 nm from the surface of the polycrystalline diamond were engineered using the microwave plasma chemical vapor deposition (MPCVD) method. A single and multiple-photon home-built confocal microscope was used to study the lifetime of NV centers in the diamond samples. The minimum detectable magnetic field sensitivity of NV sensors has been calculated theoretically and compared to the inductive pick-up coil. Lastly, we present ideas on how quantum sensors will be integrated with MRIs.

The results obtained from the fabrication of quantum sensor showed the formation of useful NV centers at a nitrogen impurity level of 0.1%. Furthermore, results from confocal microscopy suggest that near-surface modification of sample is needed to maintain optical life-time and photo-stability of negatively charged centers. Also, theoretical sensitivity calculations indicate that a reasonable choice of photon-collector will improve the magnetic field sensitivity of quantum sensor beyond the conventional limit.

The results obtained are important as a step towards the development of quantum sensors for low-field MRIs.

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## Modelling for An Intelligent Aerospace Tracking System

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In a dense aircraft surveillance environment, radar tracking of maneuvering aircraft is difficult due to the problem of discriminating against nearby target reports in the subject of multi-target tracking has applications in both military and civilian areas. The foremost difficulty in the application of the correlation process.

A tracking algorithm operating in a dense target environment is described. The algorithm provides a method for fast maneuver track adaption with relatively good discrimination against false report correlations. To further complicate the algorithm design issues, the system is nearly not observable.

A generalized intelligent Model is given for an aerospace tracking system including the jamming conditions. We illustrate our results using a computer model that simulates a typical traffic environment that may be seen in many of aerospace applications. The key performance characteristics of the designed algorithm is the flexibility for adaption to other tracking environments and incorporation into existing tracking designs.

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## **Differential Games and Singular Surfaces**

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The rules of differential games depend on the assumptions under which the players are controlling their strategies, Refs. [1,2], the question arise to what extent are the players can control their strategies if there exist singular surface? In his pioneering works Isaacs, Ref. [3] points out that the playing space of differential game will usually be divided into number of regions separated by singular surfaces. In the interior of each region the value function V(x) is twice differentiable and the" Main Equation" as well as the" Path Equations" apply.

Across the singular surfaces the gradient of V(x)usually be discontinuous and sometimes also V(x) itself. We give the game's value and the conditions for the minimax problem with which the Hamiltonian is constructed for the necessary conditions for saddle point existence. This research gives new approach for the solution of certain types of singular surfaces in differential games. Special attention will be paid to some types of singular surfaces such as Transition Surface, Universal Surface, and Dispersal Surface and how the player strategies will be affected in Two Person Zero-Sum Differential Games.

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## A Frequency-Dependent Meteorological Impulse Response Model for Accurate Water Level Prediction

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Accurate current and predicted sea water level information is a key element for safe marine navigation in shallow waters as well as for other marine operation. Sea water level prediction was conventionally carried out using various methods such as harmonic analysis method [1], wavelet network model with meteorological data effect in time domain [2] and hybrid harmonic analysis and wavelet network model for sea water level prediction [3]. With the harmonic method, the sea water level data series collected at a tide gauge is analysed to provide the amplitudes and the phases of all the embedded harmonic tidal constituents. These tidal constituents are employed to predict the sea water level. Based on the number of constituent amplitudes and phases considered in the prediction model, different levels of accuracies can be expected. Ideally spanning a period of more than 18.6 years of tide gauge data records are required to obtain the ideal accuracy, however in practice one year of data records are used to develop the harmonic analysis model [4].

The meteorological effect was investigated in time domain by El-Diasty and Al-Harbi (2015). It was shown that the meteorological effect using time-domain model could improve the prediction accuracy. However, the time domain meteorological data might contain no physical components that can only be discovered in frequency domain in forms of unexpected and sudden spikes (artifacts), which have no physical meaning [5]. Therefore, the frequency-domain model response model is considered as more robust model when compared with time-domain model.

This paper develops a frequency-dependent meteorological response model for accurate water level prediction. Sea water level data from several tide gauges are used to develop and validate the proposed model. To further validate the proposed model, a comparison is made between the proposed frequency-dependent meteorological response model for accurate water level prediction and the harmonic analysis-based model. It is found that the developed rigorous frequency-dependent meteorological response model outperforms the time-domain model and the paper will show the concluding results the findings.

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### Portfolio Optimization under Regulatory Constraints.

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In the current low interest-rate and highly-regulated environment investing capital efficiently is one of the most important challenges insurance companies face. Certain quantitative parts of regulatory requirements (e.g. Solvency II in Europe, LICAT in Canada) result in constraints (*K*) on the investment strategies ( $\pi(t)$ ) that are continuously linked to the portfolio wealth (V(t)), for example, in a Solvency II setting we have:

$$K(t, V(t), L) := \left\{ \pi(t) \in \Re^d, \frac{V(t) - L}{V(t)} \ge \sqrt{(B\pi(t) + v)^T W^T C W(B\pi(t) + v)} \right\},\tag{1}$$

where W, B and C, v, L represent regulatory and market parameters respectively.

This talk is mostly based on our recent paper [Escobar et al. (2018)] that mathematically describes the implications of Solvency II constraints on the investment strategies of insurance companies in an expected utility framework with a focus on the market risk module. For this constrained expected utility problem, we define a two-step approach that leads to closed-form approximations for the optimal investment strategy. This proposal uses first passage time solutions to circumvent the technical difficulties encountered when directly applying the convex duality approach in [Cvitanic and Karatzas (1992)]. The impact of such constraints on the asset allocation and the performance of these strategies is assessed in a numerical case study.

We will also describe alternative approaches currently under development to solve this type of constrained problems in closed-form using unconstrained solutions.

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## Spatially explicit models for forest-grassland mosaics: Exploring climate change scenarios

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Mosaic ecosystems, such as forest-grassland mosaics, consist of multiple land-states existing in close proximity. Natural forest and grassland are alternative stable states for the ecosystem, appearing as distinct spatial clusters. Changing environmental conditions, along with feedback loops and ecological thresholds, influence the system's response to disturbances, causing the proportion of each land-state to vary temporally and spatially. Forest-grassland mosaics occur around the globe; from the Southern Brazilian highlands, to India's South Western Ghats and the Jos Plateau of Nigeria.

These mosaics are endangered due to the conversion of both forest and grassland into agricultural land. Several authors have developed models which provided insights into the impacts of anthropogenic activities, such as deforestation, on mosaic ecosystem dynamics [1, 2]. However, in addition to these direct impacts, it is crucial to consider the effects of anthropogenic climate change; something not addressed in previous models. Mosaics are expected to experience climactic changes as a result of increasing atmospheric CO<sub>2</sub> levels. Ecosystem dynamics, impacted by these shifting conditions, may result in changes to the make-up of mosaics. Future conservation efforts will require not only an understanding of the natural dynamics of these systems, but of the impact of external anthropogenic drivers.

We construct a spatially explicit agent-based model of a forest-grassland mosaic, parameterised for Southern Brazilian Campos-Araucaria mosaics. Using projected changes in atmospheric  $CO_2$  concentration, as well as local temperature and precipitation data, we estimate changes in temperature and precipitation for this region up to the year 2500 and investigate how system dynamics may be altered over the coming centuries [3, 4]. Simulations using these temporally-varying dynamics are used to explore the effects of anthropogenic climate change on forest-grassland mosaics.

Preliminary results suggest that forest expansion could occur in these regions, with the extent and speed of forest cover increase determined by the  $CO_2$  trajectory followed. Additionally, the spatial structure of mosaics may be impacted by climate-driven changes in ecosystem dynamics. Through the development of this model, and analysis of spatio-temporal output from climate change simulations, we obtain further insight in to the dynamics of forest-grassland mosaics, and how they could change as we move further into the Anthropocene.

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## Fourth–Order Orthogonal Spline Collocation Methods for Two-Dimensional Helmholtz Problems with Interfaces

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We consider the use of orthogonal spline collocation (OSC), also known as spline collocation at Gauss points, for the solution of Helmholtz problems of the form

$$u_{xx} + u_{yy} + \omega^2 u = f(x, y), \quad (x, y) \in \Omega,$$
  
$$\mathscr{B}u = g(x, y), \quad (x, y) \in \partial\Omega$$

where  $\Omega$  is the unit square  $(0,1) \times (0,1)$ , with boundary  $\partial \Omega$ , and  $\omega^2$  is piecewise constant or a piecewise continuous function. The operator  $\mathcal{B}$  is the identity operator for Dirichlet boundary conditions and the normal derivative when Neumann boundary conditions are specified. Robin boundary conditions may be imposed on the sides x = 0 and x = 1. Recently, high order (that is, order three or four) compact finite difference methods have been developed for the solution of this problem with Dirichlet boundary conditions and with a vertical interface at  $x = x_{\ell}$  such that

$$\boldsymbol{\omega}^{2} = \begin{cases} \boldsymbol{\omega}_{-}^{2}, & 0 \leq x < x_{\ell}, & 0 \leq y \leq 1, \\ \boldsymbol{\omega}_{+}^{2}, & x_{\ell} \leq x \leq 1, & 0 \leq y \leq 1; \end{cases}$$

see, for example, [1, 2]. For such a problem, while u and  $u_x$  are continuous across this interface, special attention must be devoted to the approximation at the interface in the derivation of high order compact finite difference methods. In comparison, standard OSC using piecewise Hermite bicubics handles the interface without any modification, no matter the boundary conditions, Dirichlet, Neumann or mixed. When u and  $u_x$  have finite jump discontinuities at the interface, OSC with monomial bases in the x direction and piecewise Hermite cubics in the y direction handles this case without difficulty. Moreover, in each case, the linear system of algebraic equations can be solved efficiently using a matrix decomposition algorithm involving FFTs at a cost of  $O(N^2 \log N)$  on an  $N \times N$  uniform mesh. The results of numerical experiments involving published examples of each type of problem exhibit not only the optimal global accuracy of OSC but also superconvergence phenomena.

Figure 1: The AMMCS Conference is organized in cooperation with SIAM and AIMS.

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## Image reconstruction using a non-local normalized graph Laplacian

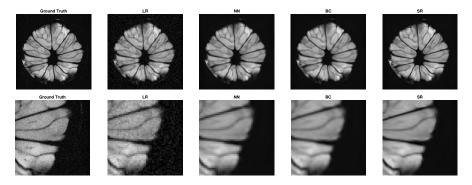
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We employ an objective function which is a sum between a sharpened data fidelity, and a regularizer denoted as the normalized graph Laplacian [1] to solve the Single Image Super Resolution problem

$$S\left(\cdot,\underline{y}\right) = \underset{x}{\operatorname{argmin}}\left(\underline{y} - \mathbf{H}\underline{x}\right)^{T} \left(I + \beta \left(I_{L} - W_{L}\right)\right) \left(\underline{y} - \mathbf{H}\underline{x}\right) + \eta \left(\underline{x}^{T} \left(I_{L} - W_{L}\right)\underline{x}\right)$$

where Low Resolution (LR)  $\underline{y} \in \mathbb{R}^{(NM) \times 1}$  is a single image represented as a lexicographical vector, a degradation operator  $\mathbf{H} = \mathbf{DB} \in \mathbb{R}^{(NM) \times (L^2NM)}$  which is constructed from a discrete local averaging operator  $\mathbf{B} \in \mathbb{R}^{(L^2NM) \times (L^2NM)}$  and discrete operator  $\mathbf{D} \in \mathbb{R}^{(NM) \times (L^2NM)}$  which down-samples an image according to a factor *L*. Filtering matrices  $W_L$  and  $W_S$  are composed via a graph based framework and hold special imaging properties such as a non-local similarity measure, a second order difference operator, preservation of DC component of images when applying filtering matrices, etc. Terms  $\beta$  and  $\eta$  are used tuned based on the amount of noise and blur of measurement  $\underline{y}$ , and vector  $\underline{n}_{\sigma}$  representing Additive White Gaussian Noise (AWGN) with standard deviation  $\sigma$  and zero mean. To synthesize High Resolution (HR) image  $\underline{x}$  the gradient of our objective is set as  $\nabla S = 0$ ; Following this to solve the system of linear equations conjugate gradient descent algorithm is utilized to find the minimum. A visual analysis is provided as well as qualitative measures including the Structural Similarity Measure (SSIM) and Peak-Signal to Noise Ratio (PSNR). The regularizer performs well for our single image inverse problem.



#### a b c d e f g h i i

**Figure 1:** Top Row: (a) Ground Truth, (b) LR image corrupted with AWGN  $\sigma = 10$  PSNR = 23.20 dB, SSIM = 0.47 (c) PSNR = 24.18 dB, SSIM = 0.58 , (d) PSNR = 24.78 dB, SSIM = 0.59 (e) PSNR = 26.74 dB, SSIM = 0.63. Bottom Row: (f) - (j) Patches of corresponding full images.

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## **Ultrahigh Frequency Mass Detection Using Nonlinear Nanowire Resonators**

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Nanoscale systems fabricated with low-dimensional nanostructures such as carbon nanotubes, nanowires, quantum dots, and more recently graphene sheets, have fascinated researchers from different fields due to their extraordinary and unique physical properties. For example, the remarkable mechanical properties of nanoresonators empower them to have a very high resonant frequency up to the order of giga to terahertz [1-2]. The ultrahigh frequency of these systems attracted the attention of researchers in the area of bio-sensing with the idea to implement them for detecting tiny bio-objects. In this paper, we originally propose and analyze a mathematical model for nonlinear vibrations of nanowire (NW) resonators with their applications to tiny mass sensing, taking into account different parameters such as temperature, piezoelectricity, electromagnetic fields, surface effects, and external excitations. The mathematical models for such nanowires are formulated using the Euler-Bernoulli beam theory in conjunction with the nonlocal differential constitutive relations of Eringen type [3].

In order to analyze the obtained nonlinear partial differential equation (PDE), we first use the Galerkin method in combination with a perturbation technique to obtain the primary resonance. After finding the primary resonance, a parametric sensitivity analysis is carried out to investigate the effects of key parameters on the sensitivity of the nanowire resonators in mass sensing. Our main premise is that attaching bio-particles to the surface of the nanowire resonator would result in a detectable shift in the value of the jump frequency. Therefore, a mathematical formula is developed based on the jump frequency to scrutinize the sensitivity of the considered nanowire resonators. Our mass sensitivity analysis aims at the improved capability of the nanowire resonator is capable of detecting tiny masses even in the order of zeptogram. As the mass of added particle increases, the frequency of NW resonator. It means that when the NW resonator is used for tiny mass sensing applications, temperature and piezoelectric potential should be monitored. It is observed that increasing electromagnetic field enhances the stiffness and also frequency of NW resonators. This is also another important factor that should be taken into account for designing nanowire resonators in sensing applications.

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## **Spatial Iterated Prisoner's Dilemma as a Transformation Semigroup**

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The prisoner's dilemma (PD) is a game-theoretic model studied in a wide array of fields to understand the emergence of cooperation between rational self-interested agents [1, 4, 5]. A pay-off matrix parametrizes the game with reward / punishment values depending on whether a player and their opponent independently choose to 'cooperate' or 'defect'. Even though mutual cooperation by both players yields a higher combined reward than mutual defection, rational players defect to maximize their individual expected reward as defection is a Nash equilibrium for two players. Iterating the game on a spatial structure with repeated interaction between players brings in a temporal aspect of long-term interaction making cooperating more attractive. Spatial structure in which multiple players interact with their neighbours as well as perturbations can play roles in influencing the distribution and dynamics of player strategies over time. where spatial clustering of similar strategies can lead to persistent cooperation [2, 3].

In this work, we formulate a spatial iterated PD as a discrete-event dynamical system where agents play the game in each time-step and analyse it algebraically using Krohn-Rhodes algebraic automata theory [6] using a computational implementation of the holonomy decomposition of transformation semigroups [7]. In each iteration all players adopt the most profitable strategy in their immediate neighbourhood. Perturbations resetting the strategy of a given player provide additional generating events for the dynamics, and with more complexity introduced by resistance to this resetting in 'stubborn' players who only adopt the reset strategy if it is more profitable. Our initial study shows that the algebraic structure, including how natural subsystems [8] comprising of permutation groups acting on the spatial distributions of strategies arise in certain parameter regimes for the pay-off matrix, and are absent for other parameter regimes. Differences in the number of group levels in the holonomy decomposition (an upper bound for Krohn-Rhodes complexity) are revealed as more pools of reversibility appear when the payoffs for cooperation and defection converge. In other regimes, the strength or weakness of the temptation to defect leads to differences in the holonomy decomposition length. Algebraic structure uncovered by this analysis can be interpreted to shed light on the dynamics of the spatial iterated prisoner's dilemma.

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#### **Robust General N User Quantum Secure Direct Communication via GHZ-Like** State

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Qua Server

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Here we will utilize the characteristic of dense coding for encrypting and transferring a successive of classical messages between N remote users with partial (Fig.1A) and complete (Fig.1B) control of the quantum server. For example, in the partial scenario, it will depend on the quantum server's publication and received user's measurement. In this scenario,  $u_1$ ,  $u_2$ , ...,  $u_N$ .  $u_1$ ,  $u_2$ , ...,  $u_{N-1}$  notifies the quantum server about his request to transfer a message to a remote user  $u_N$ . The quantum server generates and distributes N particles of N + 1 particles GHZ – like state |GHZ –  $Like >_{1....N} = |GHZ - Like >_{1...N} = \frac{1}{2} \left( |\underbrace{000 \dots 0}_{N-1} \underbrace{0}_{Q} \underbrace{0}_{N} > + |\underbrace{000 \dots 1}_{N-1} \underbrace{1}_{Q} \underbrace{1}_{N} > + |\underbrace{100 \dots 0}_{N-1} \underbrace{1}_{Q} \underbrace{1}_{N} > + |\underbrace{100 \dots 1}_{Q} \underbrace{1}_{Q} > \right).$ to  $u_{1}, u_{2}, \dots, u_{N}. u_{1}, u_{2}, \dots, u_{N-1}$  selects an arbitrarily subset of  $|GHZ - Like >_{1....N}$  and preserves it confident. Moreo-

ver, creates a random sequence bits string of transferred ordinary message. Thereafter, each user performs its unitary transformation (Ŭ<sub>1</sub> ⊗ Ŭ<sub>2</sub> ... ⊗ Ŭ<sub>N-1</sub>) Ŭ corresponds to four Pauli operations{ I, X, Y, Z} along with his ordinary message. Afterwards, the selected GHZ – Like states will be encoded in accordance with both  $u_1$ ,  $u_2$ , ...,  $u_{N-1}$  transmitted sage. Afterwards, the selected GHZ – Like states will be choosed in accordance in accordance in a selected in the selected GHZ – Like  $>_{1'...N'} = \frac{1}{\sqrt{2}} \left( \underbrace{|GHZ >_{N'}}_{u_{1},...,u_{N}} \underbrace{|\pm >_{Q}}_{Quantum} \pm \underbrace{|GHZ >_{N''}}_{U_{sers}} \underbrace{|\pm >_{Q}}_{U_{sers}} \pm \underbrace{|GHZ >_{N''}}_{U_{sers}} \right)$ 

$$\underbrace{|\pm>_{Q}}_{uantum} ) \text{ where } \underbrace{|GHZ>_{N'}}_{U_{1},\dots, U_{N}} \text{ and } \underbrace{|GHZ>_{N''}}_{U_{1},\dots, U_{N}} \text{ are one of stated GHZ states. Next, } |GHZ-Like>_{1'\dots N'} \text{ transferred to } u_{N}, u_{N}$$

applies N – GHZ measurement on his particle and  $u_1$ ,  $u_2$ , ...,  $u_{N-1}$  particles. Then, quantum server computes the status of his particle according to x basis  $\{+, -\}$  and publishes his measurement outcomes.  $u_N$  employs his measurements' and the quantum server's publication for restoring the authentic transmitted secret message by  $u_1, u_2, ..., u_{N-1}$ . GHZ - like state is robust against loss of any single qubit. That is, if a particle is lost in the GHZ - like state, the remaining particles still have an entanglement relationship between each other.

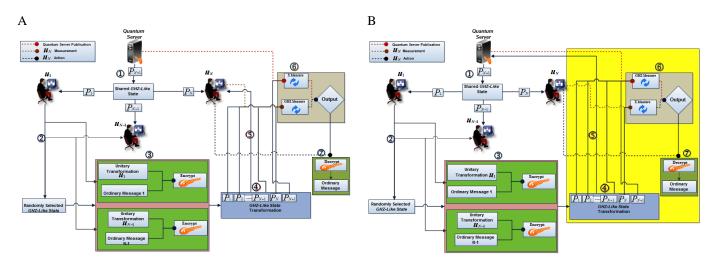


Figure 1: (A) Generalization of Communication Process between N Remote Users with Partial Control of Quantum Server (B) with Full Control of Quantum Server "Yellow box indicated the difference between partial and complete control process"

#### The inverse problem and applications

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The inverse problem of the calculus of variations addresses the question of whether or not a system of second order ordinary differential equations (SODE for short) is equivalent to a regular Lagrangian system. It dates back to the end of the 19th century, at which time only the one-dimensional case was understood. In 1941 the Fields medalist J. Douglas gave a classification for two-dimensional systems [1]. After that no other dimension has been classified, but deeper geometric understanding of the problem allowed the extension of some of the cases in Douglas' classification to arbitrary dimension [2]. In [1] Douglas also introduced the Helmholtz conditions, a well-known set of algebraic and PDE equations which are necessary and sufficient for a SODE to be variational, that is, equivalent to a regular Lagrangian system. These conditions are written in terms of a multiplier matrix which corresponds to the Hessian of the sought Lagrangian with respect to the velocities, and they were used by Douglas in order to derive his classification.

In [3] Bloch, Leonard and Marsden presented a strategy to explicitly construct feedback controls that would stabilize certain mechanical systems with symmetry. The idea is to modify the Lagrangian of the given mechanical system in a prescribed way in order to obtain that the original controlled Lagrangian system is equivalent to the Lagrangian system corresponding to the new Lagrangian, which will depend on some parameters. Sufficient conditions to achieve this goal are referred to as matching conditions. I will present two different applications of the inverse problem to this control problem.

First, by using the Helmholtz conditions in [4] we are able to recover the matching conditions from [3] (since the Helmholtz conditions are necessary and sufficient conditions for existence of a regular Lagrangian), but further we can derive new matching conditions for a particular class of mechanical systems. It turns out that for this class of systems we obtain feedback controls that only depend on the configuration variables.

In [5] we use the other main tool, Douglas' classification, in order to obtain new stabilizing controls for a class of two-dimensional mechanical systems. The main difference in the strategy with respect to [3] is that now we do not impose any specific form for the new Lagrangian, but work instead among a certain class of controls. This approach is so far restricted to dimension two since it relies on Douglas' results, but it uses one of the cases of the classification which is always variational in arbitrary dimension, raising the possibility of a generalization.

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# Local Fourier Analysis for Overlapping Additive Block Relaxation Schemes

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Multigrid methods are popular solution algorithms for many discretized PDEs, either as standalone iterative solvers or as preconditioners, due to their high efficiency. However, the choice and optimization of multigrid components is crucial to the design of optimally efficient algorithms. Local Fourier analysis (LFA) is a useful tool to predict and analyze the convergence behavior of a relaxation scheme or multigrid method for discretized PDEs. In this talk, we develop a framework for LFA of overlapping block relaxation schemes, for which classical LFA cannot be used directly. In particular, we show that such additive block relaxation schemes satisfy an invariance property; that is, the Fourier modes form a basis for invariant subspaces of the scheme. Furthermore, we build a general structure of how to compute the LFA smoothing and two-grid convergence factors for overlapping additive cell-wise relaxation. Finally, we use the Laplacian, grad-div equation, and the Stokes equations as demonstrative examples.

# The generalized wavelet convolution associated with the linear canonical transform

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The linear canonical transform (LCT) plays an important role in modern optical and signal processing domain, Many operations, such as the Fourier transform (FT), the fractional Fourier transform (FRFT), the Fresnel transform (FRST), time shifting and scaling, frequency modulation are all special case of the LCT. The *n*-dimensional LCT is defined as follows [1],

$$\hat{f}(q) = [\mathscr{C}(M)f](q) = \int_{\mathbb{R}^n} C(M)(q,q')f(q')\,\mathrm{d}q' \tag{1}$$

where

$$C(M)(q,q') = C \cdot e^{i(\frac{q^T D B^{-1} q}{2} - q^T B^{T^{-1}} q' + \frac{q'^T B^{-1} A q'}{2})},$$

and

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, M^{\mathsf{T}}JM = J, J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, C = \frac{e^{(-\frac{in\pi}{4})}}{(\sqrt{2\pi})^n \sqrt{\det(B)}}$$

The wavelet transform (WT) is another important tool for time-frequency analysis [2] in signal processing, which has found many applications in time-dependent frequency analysis, data compression, etc. The *n*dimensional WT with respect to wavelet  $\psi \in L^2(\mathbb{R}^n)$  is defined by

$$W_{\psi}f(b,a) = \int_{\mathbb{R}^n} f(t)\overline{\psi_{b,a}(t)} \,\mathrm{d}t, b \in L^2(\mathbb{R}^n), a > 0 \quad \text{and} \quad \psi_{b,a}(t) = |a|^{-n}\psi(\frac{t-b}{a}) \tag{2}$$

However, the signal analysis capability of the WT is limited by the time-frequency domain. Although, the linear canonical transform can perfectly represent signals in the linear canonical transform domain, but it fails in obtaining local information of the signal. As a generalization of the WT, the linear canonical wavelet transform(LCWT)[3] combines the advantages of the WT and the LCT, hence, the LCWT may be potential usefulness in the applied mathematics and signal processing community, to the best of our knowledge, no studies about the *n*-dimensional WT related to the LCT have been reported.

In this paper, we will propose definition and properties of the *n*-dimensional linear canonical wavelet transform, which not only inherits the advantages of multiresolution analysis of the WT, but also has the capability of signal representations in the linear canonical community. The *n*-dimensional wavelet convolution product by using the theory of wavelet transform and linear canonical transformation tool are also obtained. Additionally, the Plancherel formula for *n*-dimensional WT associated with the LCT is derived. And *n*-dimensional generalized wavelet convolution and generalized wavelet translation using the linear canonical transform are obtained.

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# **Convolutional Neural Network Modelling for Polysomnography Data of Obstructive Sleep Apnea Diagnosis**

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Identifying the sleep problem severity from overnight polysomnography (PSG) recordings plays an important role in diagnosing and treating sleep disorders such as the Obstructive Sleep Apnea (OSA), which affects people especially children's health. This analysis traditionally has been done by experts manually through visual inspections, which can be tedious, time-consuming, and is prone to subjective errors. Currently, there are many machine learning solutions used for analyzing and classifying PSG data. One of the proposed solutions is to use deep learning architectures such as Convolutional Neural Network (CNN) where the convolutional and pooling layers behave as feature extractors and some fully-connected (FCN) layers are used for making final predictions for the OSA severity classes. In this project, a CNN architecture with 1D convolutional layers and FCN layers for classification is presented in Figure 1. The PSG data for this project are from the Cleveland Children's Sleep and Health Study database and classification results confirm the effectiveness of the proposed CNN method. The proposed model of 1D CNN achieves excellent classification results without manually preprocessing PSG signals such as feature extraction and feature reduction.

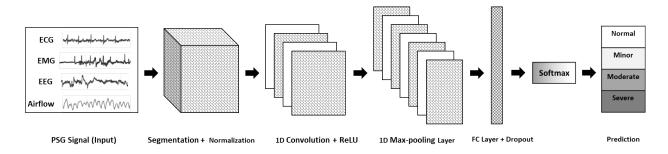


Figure 1: The flow chart of 1D-CNN

# Fundamental solutions of a fractional equation with Laplace operator

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In this work we obtain the first and second fundamental solutions (FS) of the multidimensional time-fractional equation with Laplace or Dirac operators, where the two time-fractional derivatives of orders  $\alpha \in ]0,1]$  and  $\beta \in ]1,2]$  are in the Caputo sense. We obtain representations of the FS in terms of Hankel transform, double Mellin-Barnes integrals, and H-functions of two variables. As an application, the FS is used to solve Cauchy problems of Laplace and Dirac type.

Keywords: Laplace operator, fractional calculus, fundamental solution.

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# Multidimensional time-fractional diffusion-wave and parabolic Dirac operators and their fundamental solutions

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In this talk, we study the multidimensional time-fractional diffusion-wave equation where the time fractional derivative is in the Caputo sense with order  $\beta \in ]0,2]$ . Applying operational techniques via Fourier and Mellin transforms we obtain an integral representation of the fundamental solution (FS) of the time fractional diffusion-wave operator. Series representations of the FS are explicitly obtained for any dimension. From these we derive the FS for the time fractional parabolic Dirac operator in the form of integral and series representation. Fractional moments of arbitrary order  $\gamma > 0$  are also presented. To illustrate our results we present and discuss some plots of the FS for some particular values of the dimension and of the fractional parameter. The results presented in talk can be found in [1].

This presentation is based on a joint work with M. Ferreira (IPLeiria & CIDMA).

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# First order system of ODE's: The role of functional boundary conditions on applications in medicine

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In this paper some existing results on first order coupled systems with functional boundary conditions are used with the intent to explore and emphasize the applicability and general aspect of functional boundary conditions. Functional boundary conditions generalize many of the usual and most common boundary conditions and 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 such as biology, medicine, chemistry, engineering, economics and explore models subject to global conditions, which could not be explored using common tools. To illustrate these features, two applications in medicine are presented. One is an application to an epidemic model of HIV infection and the other is an application to the thyroid pituitary homeostatic mechanism.

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# Key performance indicators and individual prediction models on kicks from the penalty spot

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In the recent years quite a few papers have been dedicated to he study of penalty kicks in soccer. With the intent of predicting the direction final outcome of the kick, several different factors have been analyzed, from kinematics, biomechanics, stress levels, individual skills and fatigue are just some of the factors. In this paper, the authors study a selected group of football players with the objective of identifying key performance indicators on kicks from the penalty spot in soccer. Using data analysis techniques via Python, several variables are analyzed, in order to identify the individual key performance drivers, with the final intent to build a predictive model for each player.

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#### The Least Prime in the Chebotarev Theorem

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The work of Bach [1] and Bach-Sorenson [2] provided the first effective (though conditional) bounds for respectively the collection of primes needed to generate the class group and the smallest prime in the Chebotarev density theorem. In both cases the result is of the form

$$c(1+o(1))(\log |D_L|)^2$$

where c is either 12 or 1 in the respective cases, and  $D_L$  is the discriminant of the field in question. These results have important applications in algorithms for computing class groups and primality testing, forming the basis for efficient algorithms. In practice though this bound does not appear tight, but little is known about the potential for improvements.

In this talk we will discuss both our work towards computationally verifying stronger results of the same type for fields of small discriminants, as well as theoretical results, discovered as a consequence of these computations, which give an infinite family of fields for which the least prime in the Chebotarev theorem realizes the lower bound

$$(1+o(1))\left(\frac{3e^{\gamma}}{2\pi}\right)^2\left(\frac{\log|D_L|\log\log\log|D_L|}{\log\log|D_L|}\right)^2.$$

This second result is discussed in detail in [3] and significantly improve on our understanding of the extent to which improvements to the result of Bach and Bach-Sorenson might be improved.

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### On Sets to Initialize the Chaos Game to Render Attractors of IFS

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The chaos game is random algorithm used to render (or draw/approximate) attractors of Iterated Function Systems (IFS). Recently [1], researchers have considered playing the chaos game to render attractors in more abstract topological spaces. Since, these topological spaces are not necessarily metrizable, the functions in the IFS may not be contractive (or even Lipschitz). Hence the classical contractive IFS framework can no longer be used and the notation of the attractor is lost in this classical sense. Thus researchers invented a number of generalizations of attractors such as the strict attractor, pointwise attractor and quasi-attractor. For each of these attractors there is a basin of attraction in which the chaos game is initialized.

In this talk we will consider IFS with lower semi continuous Hutchinson operator (this will allow for discontinuous functions in the IFS) and present a number of results involving the basins of attraction. Including the definition for the largest basin of attraction (the largest set in which the chaos game can be initialized and potentially render the attractor with probability one). Under additional assumptions we show that the chaos game does in fact render quasi attractors (the most general of the 3 attractors mentioned).

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#### Model identification for blood sugar levels

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As medicine is pivoting from diagnosis to prediction, models of "healthy" will be needed to predict the onset of "disease". Healthy physiological systems are defined by homeostasis: the maintenance of specific variables, such as core temperature, blood pressure, body mass and glucose level within an optimal range, regardless of external stimuli. Homeostasis is, in essence, a control system. The majority of medical studies of this control system are conducted on sick rather than healthy subjects. In contrast, healthy states are often defined merely as values or ranges, not as properties of homeostatic time series or models of the control system at work. Furthermore, while models of physiology exist, these tend to be rather complicated as measured, for instance, by the number of variables and parameters, and describe a multitude of elementary biophysical processes rather than the resulting control strategy itself. As a consequence, an opportunity exists around modeling the homeostatic control systems of healthy subjects.

Playing into this opportunity is the ever increasing amount of homeostatic data that is becoming available due to the miniaturization of sensors and their integration with everyday electronics like watches and phones. To mention a few examples: heart rate measurements can be taken and transmitted by watches and core temperature can be estimated from the infrared sensitivity of cameras in tablets. The overarching goal of this study to develop parsimonious models of the control system regulating such streams of homeostatic data.

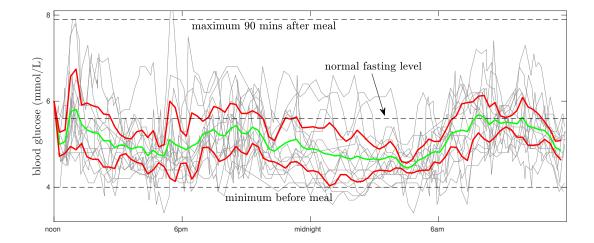


Figure 1: Example of a blood glucose time series. Shown is 14 days of measurements taken every 15 minutes. The green line denotes the daily average and the red lines denote the average plus and minus one standard deviation. The dashed line indicate some target levels of the underlying control system.

Armed with a predictive model, one may be able to extract early warning signals from real-time data. This, in turn, could greatly improve the efficiency of patient care. Effectively, understanding and modelling the homeostatic control system based on measured data will allow us to develop secondary biomarkers for the onset of pathological states. Often the primary, or *gold standard*, indicator is intrusive (e.g. taking blood samples), expensive (e.g. MRI scans) or time-consuming (e.g. requiring a doctor's visit).

In this pilot study, we examine time traces of blood sugar levels obtained with an inexpensive patch worn by the subject over the course of two weeks. Around 50 healthy individuals were recruited by Klick Research Labs for this study, and the data are currently being processed. The data yield a running average over a few minutes, taken every fifteen minutes. An example time series from a single subject is shown in Fig. 1. Two features are evident: there is a fair amount of scatter due both to measurement error and variations in the subject's daily schedule and there is a clear circadian rhythm, with an average low between midnight and 6am and peaks at meal times. A third feature becomes evident when comparing the time series to the minimal before-meal, the maximal after-meal and the normal after-sleep levels, indicated with dashed lines. There is an active control system at work to quickly restore the blood sugar concentration to safe levels.

The purpose of this study is to model this active control without considering the physiological details of the control mechanism. We will investigate the hypothesis that a phenomenological model of low complexity – in particular having few tunable parameters – can describe blood sugar control across patients and life styles. Such a model would be complimentary to brute-force data modelling with machine learning techniques [1] and, potentially, aid in the construction of robust algorithms to detect anomalies in streams of blood sugar measurements.

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### How to make spin and lattice dynamical together

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A coupled spin and lattice dynamics approach is developed which merges on the same footing the dynamics of these two degrees of freedom into a single set of coupled equations of motion. Our discussion begins with a microscopic model of a material in which the magnetic and lattice degrees of freedom are included. This description comprises local exchange interactions between the electron spin and magnetic moment as well as local couplings between the electronic charge and lattice vibrations. We construct an effective action for the spin and lattice variables in which the interactions between the spin and lattice components is determined by the underlying electronic structure. In this way, we obtain expressions for the electronic contribution to the inter-atomic force constant, the isotropic and anisotropic spin-spin exchanges, as well as the electronically mediated coupling spinlattice exchange. The last of these exchanges is provides a novel description for coupled spin and lattice dynamics. It is important to notice that our theory is strictly bilinear in the spin and lattice variables and provides a minimal model for the coupled dynamics of these subsystems. Questions concerning time-reversal and inversion symmetry are rigorously addressed and it is shown how these aspects are absorbed in the tensor structure of the interaction fields. Using our novel results regarding the spin-lattice coupling, we can provide simple explanations of ionic dimerization in double anti-ferromagnetic materials, as well as, charge density waves induced by a non-uniform spin structure. In the final parts, we construct a set of coupled equations of motion for the combined spin and lattice dynamics, reduced to a form which is analogous to the Landau-Lifshitz-Gilbert equations for spin dynamics and damped driven mechanical oscillator for the ionic motion, however, comprising contributions that couple these descriptions into one unified formulation. We provide Kubo-like expressions for the discussed exchanges in in terms of integrals over the electronic structure and, moreover, analogous expressions for the damping within and between the subsystems.

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# Towards hierarchical TDA learning

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Many approaches to learning on graphs have appeared in the last two decades. Much of this work has been in terms of *graph kernels* (e.g. early works [1, 3]) and this continues to be an active area of research. Hierarchical and compositional aspects have also been a recurring theme in learning on discrete structures such as graphs, from seminal work of Haussler [2] to the highly active field of *graph neural networks* (c.f. [4] an early proponent). The latter takes inspiration from deep learning where building a representation is bound into the learning process itself. A natural extension to learning on graphs, just beginning to receive attention, is learning on objects from TDA, such as persistence diagrams or even just simplicial complexes. In this informal talk I will discuss some work in progress.

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### Group Fairness for the Allocation of Indivisible Goods

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Mathematical models of fairness have been proposed and studied in the context of resource allocation since the work of Steinhaus [1], but fairness has been a subject of interest since millennia. Much of the existing literature on fair division focuses on notions of individual fairness. For instance, when allocating divisible goods (such as a piece of land or a cake) to a set of agents, a classic notion of individual fairness is *envy-freeness* [2], which requires that no agent prefer the allocation of another agent to her own allocation. When allocating indivisible goods, envy-freeness cannot be guaranteed; hence, its relaxations — such as envy-freeness up to one good [3, 4] — have been studied.

We observe that an algorithm satisfying such individual fairness notions can still treat *groups of agents* unfairly, with one group desiring the goods allocated to another. Our main contribution is a notion of *group fairness*, which is strictly stronger than individual fairness and provides a fairness guarantee to all possible subgroups of agents. In contrast, most contemporary notions of group-level fairness proposed in the machine learning literature are weaker than individual fairness (as they only ensure that outcomes are fair *on average* across groups) and typically require the groups to be specified in advance (e.g. in terms of protected demographic attributes).

We show that for divisible goods, our notion of group fairness can be achieved exactly. For indivisible goods, group fairness (like individual fairness) cannot be satisfied exactly; hence, we introduce two "up to one good" style relaxations. We prove that checking whether a given allocation satisfies group fairness up to one good is a coNP-hard problem. On the positive side, we find, somewhat surprisingly, that certain local optima of the Nash welfare function satisfy both relaxations and can be computed in pseudo-polynomial time using local search. We provide an interpretations of such local optima in terms of an approximate market equilibrium characterization.

Our experiments using real data suggest that in practice these local optima can be computed very quickly, and often provide stronger fairness guarantees than suggested by the theory.

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# **Efficiency of Contaminant Removal in Ceramic Water Filters using Bacterial Biofilms**

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In many developing countries access to clean drinking water is not always readily available, resulting in the need to collect water from other locations. By collecting water elsewhere and returning home, there is a high chance that the source water is contaminated. Many point-of-use water filters have been used in the treatment of contaminated source water, with the most widely selected water filter being ceramic water filters (CWFs). CWFs are constructed of clay, sand, and organic material, such a rice husks and sawdust. During the firing process, the organic material is burned away and small pore spaces remain in the bed of the pot and can act as a filter. The pores help control the flow rate of water (typically 1-3 L/hr) through the filter and remove contamination from the source water.

In this work we investigate point-of-use CWFs by reformulating an existing multi-scale biofilm model that has been developed for porous medium applications. The reactor model is described by a stiff system of quasilinear hyperbolic balance laws, which are studied numerically. The model considers processes related to hydrodynamics and transport of a single target contaminant, growth/death of bacteria (both wall attached, in the form of biofilms, and suspended bacteria), and mass exchange between the biofilm and suspended bacteria via attachment and detachment. With this model we investigate the influence of water height in the CWF and refill frequency on the amount and quality of recoverable water.

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#### A DFT Study of Small Gold Superatoms

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Recently, it was discovered that certain stable metal clusters could imitate the chemical property of an atom in the periodic table of the elements, and the term superatom was introduced. "Inert" superatoms have a closed-shell electron count (2, 8, 18, 20) that differs from the atomic series (2, 10, 18). This superatomic electron counting rule is an effective tool for interpreting geometrical structures and stability, as well as the chemical nature of cluster compounds. A principle goal of this research project is to gain an understanding of how ligands influence small gold superatoms as a function of the number of gold atoms and the number of ligands, while taking into account the geometrical arrangement of atoms and charge of the gold nanocluster. A ligand of interest is the linear X-Au-X (X=F, Cl, Br, and I) fragments, which I have discovered can arrange into staple motifs similar to the gold-thiolate staples reported in the literature.<sup>1</sup>

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## Modelling the influence of campaign contributions and advertising on US Presidential elections

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We provide a stochastic electoral model of Presidential election where candidates use the campaign contributions they receive from special interest groups (SIGs) to run their electoral campaign. Prior to the election, candidates announce their policy platforms and advertising (ad) campaigns and use the contributions of SIGs to generate two SIG valences that enhance their electoral chances. Voters have preferences over candidates' policies relative to their ideal policy and over candidates' ad messages relative to their ideal message frequency, their campaign tolerance level. Voters' choices are also influenced by candidates' endogenous SIG valences: one associated with candidates' policy platform, the other with their ad campaign. Citizens' choices also depend on their sociodemographic characteristics and on candidates' traits and competences. Candidates' critical policy and ad campaign are a weak local Nash equilibrium (LNE) of the election if the expected vote shares of all candidates are greater than their corresponding pivotal vote shares. In LNE, candidates' policy and ad campaign balance the SIG and electoral pulls. If the expected vote share of at least one candidate is lower than its pivotal vote share, then the critical campaigns are not a LNE of the election.

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#### **Inverse Problems for Perturbed Mixed Variational Equations**

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Collage-based Inverse Problems can be viewed in terms of the approximation of a target element in a complete metric space by the fixed point of a contraction mapping [1]. In fractal imaging this result has been used to approximate a target image by the fixed point (image) of a contractive fractal transform.

These ideas have been extended to inverse problems for ordinary differential equations in recent papers [2] [4] [8] [9].

The study of mixed variational formulations as well as its numerical treatment is a well stated area of numerical analysis and it is based on the Babuska–Brezzi theory [3] [7] and some of its generalizations. In this paper we consider a perturbed problem appearing when including a new bilinear form, small in a sense [5] [6]. We establish a result of existence of a unique solution for such a problem, introduce the corresponding Galerkin method and analyze an associated inverse problem.

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#### Numerical study of the geometry of a vertical U-tube ground heat exchanger

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Ground source heat pump systems consist of ground heat exchangers with fluid circulating inside pipes located in the ground (laid in a trench or as a borehole). The geometry of the heat exchange pipes plays a significant role in the efficiency and operation of Ground Heat Exchangers (GEHs). The piping system of a U-tube GEH depends on parameters such as the borehole radius, the inner and outer pipe radii, annular space, heat transfer coefficients, the number of boreholes,  $\Delta T$ , and fluid mass flow rate. Moreover, the lengths of the pipes may be different for heating or cooling loads [1].

In this study, a numerical simulation of a vertical U-tube GHE is presented. A quadratic mesh was generated for the pipe-annulus-soil system, and the heat transfer simulated using a Computational Fluid Mechanics (CFD) modeling approach. The details of the numerical mesh geometry were provided by an optimization method. The analysis of heat transfer from the numerical simulation provides useful information for determining the optimum length of the heat transfer pipes and can be extended to the optimum management method for an array of vertical GHEs in a heat repository designed for various sizes and time scales. Figure 1 shows an example of temperature distribution in the borehole.

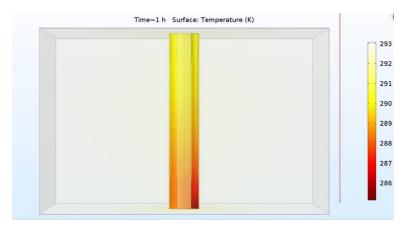


Figure 1: Temperature distribution inside the borehole.

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## Numerical investigation of VAWT airfoil shapes on power extraction and selfstarting purposes.

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The effects of airfoil shapes on the power coefficient and the torque coefficient have been studied for an Htype Darrius vertical axis wind turbine (VAWT). Different types of airfoils were analyzed, and eight of them were selected and divided into two groups. The first group includes the airfoils with camber while the second group has symmetric geometries [1]. The focus of the current study is on two-blade VAWTs because they have higher power coefficient than three or four blades VAWTs [2]. The two-blade VAWTs with selected airfoils were simulated with Computational Fluid Dynamic (CFD) method, and k- $\omega$  SST was used as a turbulence model and then grid independency was checked. The numerical results show which airfoil produces the highest power coefficient and which one has the best torque coefficient.

The power coefficient,  $C_p$ , is defined as a ratio of the produced power, P, to the maximum available power.

$$C_p = \frac{P}{\frac{1}{2}\rho A V_0^3},\tag{1}$$

where  $\rho$  is the density of the air and A is the projected area of the rotor and  $V_0$  is the upstream wind speed. The torque coefficient,  $C_t$ , is defined as a ratio of the power coefficient to the tip speed ratio.

$$C_t = \frac{C_p}{\lambda},\tag{2}$$

where  $\lambda$  is the Tip Speed Ratio (TSR).

The numerical investigation indicates that the cambered airfoils produce the highest static torque and are qualified for self-starting purposes. In addition, the symmetric airfoils produce the highest power coefficient and are qualified for power extraction, Figure 1.

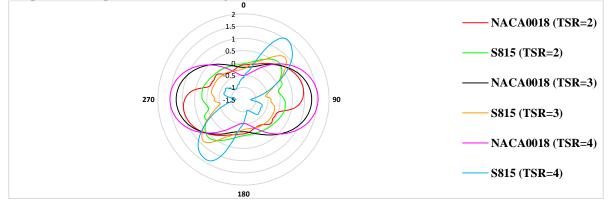


Figure 1: Power Coefficient of Two Blades VAWT in different TSR

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# Adaptive GPU accelerated discontinuous Galerkin method applied to solution of von Neumann paradox

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Adaptive mesh refinement is used to concentrate mesh cells in order to resolve fine features of the solution. We present novel algorithms for run-time, cell-based adaptive mesh refinement on unstructured meshes of triangles on graphics processing units (GPUs) for hyperbolic problems. Our implementation makes use of improved memory management techniques and a coloring algorithm for avoiding race conditions. The algorithm is entirely implemented on the GPU, with negligible communication between device and host. We show that the overhead of the AMR subroutines is small compared to the high order solver and that the proportion of total runtime spent adaptively refining the mesh decreases with the order of approximation.

We demonstrate performance of our algorithm by presenting a solution to a shock reflection problem that addresses the von Neumann triple point paradox with an accurately computed triple point location. This is a computationally challenging problem involving cell size varying by seven magnitudes. We present fully adaptive computations on an unstructured mesh, which allows us to obtain a more accurate position of the triple point than previously reported. We are also able to resolve several self-similar reflection patterns that result from the oblique reflection of a shock against a wedge.

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# Simulation of wind patterns on Sub-Antartic Marion Island using Computational Fluid Dynamics and measured wind data

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A need was identified to have reliable quantitative wind pattern data for Marion island in the study of terrestrial ecology (fauna and flora) on this well-preserved and remote location. A measurement campaign was launched in 2018 consisting of 17 sonic anemometer stations, each measuring at two heights, as shown in Figure 1; to be extended in 2019 with two additional stations in areas requiring more resolution.

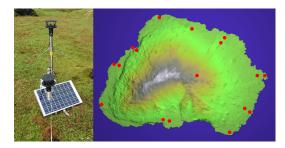


Figure 1: Example station setup (*left*) and approximate locations across Marion Island (*right*).

These data are available for the calibration and setup of Computational Fluid Dynamics (CFD) simulation of island wind patterns. The aim of the present study is to simulate air flow across Marion Island's topography using CFD. Intermediate steps include: using topographical data scanned using drones to identify surface features that require sufficient mesh resolution (thereby aiding the accurate prediction of wind patterns); converting file formats to those required by CFD meshers; determining initial and boundary conditions from measured wind location data; simulating wind patterns for dominant wind directions; etc.

To validate the process, the well-known Bolund island case study is used [1][2]. The goal of the series of simulations contained in the final paper is to provide a baseline set of wind patterns that can serve as a reference for future climate change impacts on ecology. Once a baseline simulation model has been created, it may be used to assess the relationship between the wind patterns and the ecological systems in the current climate. It is then possible to computationally simulate wind flows at additional wind directions, thereby assessing the impact of a change in dominant wind direction on ecological systems on Marion Island.

**Keywords:** Simulation, Computational Fluid Dynamics, Wind Patterns, Atmospheric Boundary Layer, Complex terrain modelling, climate change.

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#### Globalized high-order methods for unconstrained optimization

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We consider the numerical solution of the nonlinear unconstrained optimization problem

$$\min_{x \in \mathbf{R}^n} f(x) \tag{1}$$

where, for our study, f is assumed to be at least three times differentiable. One of the best-known methods to solve (1) is Newton's method, which has been studied since the 17th century. A key feature of Newton's method is the use of second-order derivatives, which results in local quadratic convergence to an isolated solution. High-order methods result in cubic convergence (or higher) to an isolated solution. While certain high-order methods, such as Shamanskii's method [2], only use second-order derivatives, the main burden of high-order methods, such as Chebyshev's [1] or Halley's method [3], is the computation of third-order derivatives. Even though the cost of high-order derivatives is high, recent progress in automatic differentiation allows simple and relatively efficient computation of derivatives that makes the study of high-order methods more interesting than ever.

We present several ideas for globalizing high-order methods mainly based on traditional trust-region schemes, but also linesearch approaches. We describe the convergence properties and report preliminary numerical results of our globalized high-order methods. We show that despite their higher cost, the globalized high-order methods can yield clear improvements over the traditional Newton trust-region method.

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# Neural Network Approaches to An Inverse Fractal Problem

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An iterated function system is defined to be the union of a finite number of contraction mappings on a complete metric space [1]. The fixed point of a contractive iterated function system is a fractal set called its attractor. Practically, we can only obtain finite approximations of the fractal through fixed point iteration. A difficult optimization problem within this field is, given some initial target set (fractal or not) to obtain an iterated function system whose attractor is close, in some measure, to it. Neural networks have demonstrated powerful optimization properties, including imaging applications. For instance, in 2015 a neural network surpassed human-level performance on object classification in the ImageNet database, one with millions of images and thousands of categories [2]. Hence, we explore neural network approaches to this inverse problem.

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# An Unconditional Improvement to the Running Time of the Quadratic Frobenius Test

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Damgård and Frandsen demonstrated an extension to the Quadratic Frobenius Test (a probable primality test) which has a reduced running time. This improvement can be extended to other versions of the test, but in general depends on the Extended Riemann Hypothesis. I will show how to achieve a speedup intermediate between the original and the new running times that does not depend on any unproven hypotheses.

# eBACOLI: Software for solving one-dimensional multi-scale parabolic-elliptic PDE systems with adaptive error control

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BACOLI is a Fortran software package for solving one-dimensional parabolic partial differential equations with separated boundary conditions by B-spline adaptive collocation methods [1]. A distinguishing feature of BACOLI is its ability to estimate and control error through the use of adaptive meshes in both space and time. We recently extended BACOLI to a Fortran software package eBACOLI to solve multi-scale parabolic PDE systems of the form of coupled systems of parabolic partial differential equations describing dynamics on a global scale with systems of ordinary differential equations describing dynamics on a local scale [2]. We now describe a further extension to eBACOLI to solve multi-scale models that also include elliptic PDEs. Results from new eBACOLI are given for various multi-scale models from the extended problem class considered.

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#### Data-based optimization for learning and control

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Recent technological advances on sensing equipment, communication networks and computational hardware have contributed to a dramatic increase in the availability and storage of data and the transmission of information both within and between the social, commercial, financial and industrial sectors. The interaction between information management systems, data transmission networks, and systems in the physical world is indeed becoming more and more prevalent in various application domains. Examples are large-scale networked systems, such as energy smart grids and intelligent transportation systems, and autonomous engineering systems, such as self-driving cars, robots for care and cure and many more. This explosion of data availability offers a wealth of new information that can be, but often not yet is, used to improve the performance, reliability and safety of such complex engineering systems.

Existing model-based controller design, estimation and optimization techniques are difficult to implement for such complex, autonomous systems since reliable models are typically unavailable. Consequently, there is a growing need for the development of data-driven methodologies for system automation and optimization. With the advent of recent developments in learning-based controller design techniques, such as machine learning, iterative learning control and extremum-seeking control, control experts are now equipped with a growing set of datadriven controller design techniques that can solve complex control problems in the absence of exact knowledge of process dynamics. These techniques provide mechanisms to exploit available data to account for the uncertain mathematical nature of the process, while still achieving performance objectives.

These leading data-driven learning control and optimization fields have evolved almost independently of each other. Some researchers have started to identify and capitalize on the potential synergies between these fields to develop new techniques and strengthen the theoretical foundations of learning. For example, machine learning techniques can deal with complex systems. However, it generally requires large data sets and lacks certificates for stability, robustness and optimality On the other hand, extremum seeking techniques, which requires more restrictive assumption, can function well with only limited (performance) data sets while providing such certificates.

In this presentation, we wish to argue the growing synergy between extremum seeking control and learning techniques. It is shown how simple control techniques can be utilized to improve the real-time performance of learning-based methodologies to achieve stability and optimality.

# Multiscale/multiphysics modeling of ocular physiology: the eye as a window on the body

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Vascular anomalies are involved in many diseases, including cardiovascular diseases, diabetes and neurodegenerative disorders. Oftentimes, the vascular damage goes on silently for many years without detection in various organs, including brain and kidneys. Thanks to its accessibility via noninvasive measurements, the eve offers a very unique opportunity for vascular assessment. However, vascular features in the eye are the results of complex interactions between factors that (i) are specific to the eye, e.g. intraocular pressure; (ii) are associated with other organs, e.g. intracranial pressure; and (iii) depend on systemic conditions, e.g. blood pressure. The complexity of the multiscale interactions among these components make it extremely difficult to single out the relative contribution of each factor experimentally. To address this challenge, we have been developing a high performance computing platform that (i) enables an integrated view of multimodal ocular imaging data; and (ii) processes the integrated data by individualizing the analysis method to the patient's specific clinical conditions. This platform is based on Feel++ [1], a finite element C++ library to solve partial differential equations (PDEs), which has been interfaced with OpenModelica, a freeware targeted to deal efficiently with ordinary differential equations (ODEs). The PDE/ODE coupling, which accounts simultaneously for local and nonlocal factors, is dealt via (i) operator splitting for the time discretization, providing modularity of the solution algorithm while preserving the physical energy at the discrete level [2]; and (ii) Hybridizable Discontinuous Galerkin (HDG) method for the PDE discretization, ensuring conservation of fluxes of mass and linear momentum at the discrete level [3].

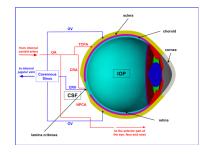


Figure 1: Schematic representation of multiscale modeling of ocular perfusion.

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# A 2D Simulation of Aqueous Humor Hydrodynamics in the Anterior Chamber by FreeFEM++

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In human eyes, the aqueous humor (300 microliters) is secreted into the posterior chamber by the ciliary epithelium, and subsequently, it escapes into the anterior chamber via the pupil. It exits the eye mainly via the trabecular meshwork (TM), and the flow rate at steady state is ~ 2.5 microliters/min. It's resistance to outflow through the TM sets up an IOP of ~15 mmHg. Since the temperature at the corneal surface is slightly lower (35 °C) compared to that at the surface of the vascularized iris (37 °C), the aqueous humor shows convective mixing in the anterior chamber. In this study, we have modeled the convection currents of the aqueous humor.

This study has modeled in the standing posture, and when lying down and looking up. Aqueous humor in anterior chamber has modeled as Boussinesq fluid.

$$\nabla \underline{v} = 0 \tag{1}$$

$$\nabla \underline{\underline{T}} + +\rho_0 \left(1 - \alpha(\theta - \theta_0)\right) \underline{\underline{g}}$$
<sup>(2)</sup>

$$\underline{P} = -p\underline{I} + \mu\nabla\underline{v} \tag{3}$$

$$\nabla J = 0 \tag{4}$$

$$J = -\kappa \nabla \theta \tag{5}$$

Our findings are useful in predicting the pharmacokinetics and optimal placement of drug delivery implants in the anterior chamber, in predicting particle velocities, deposition of inflammatory cells on the endothelial surface.

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# New mixed finite-element methods for the biharmonic problem

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Fourth-order differential operators often appear in mathematical models of thin films and plates, and pose significant challenges in numerical simulation over equations governed by more familiar second-order operators. In this talk, we present two three-field mixed finite-element formulations for the biharmonic problem, with some focus on what happens with different boundary conditions. These formulations are based on introducing the gradient of the solution as an explicit variable, constrained using a Lagrange multiplier. As a result, the problem is rewritten as a saddle-point system, requiring specialized analysis of the finite-element discretization. Here, I will discuss the analysis of well-posedness and accuracy of both formulations, as well as experimental results to be compared with the analysis.

### Planar Central Configurations of the N-Body Problem with a Homogeneous Potential

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The classical Newtonian *N*-body problem is concerned with the motion of *N* point particles with non-negative masses  $m_i$ , interacting via a central potential *U* are given by:

$$m_i \ddot{q}_{i;j} = \frac{\partial U}{\partial q_{i;j}}, \quad i \in \{0, \dots, N-1\}, \quad j \in \{1, \dots, d\}$$

where  $q_i \in \mathbf{R}^d$  is the position of particle *i* with components  $q_{i;j}$ , and

$$U = \sum_{i < k} m_i m_k / r_{i,k}^{A-2}$$

is the potential with a real parameter A > 2, and  $r_{i,k}$  is the distance between  $q_i$  and  $q_k$ . In the Newtonian case A = 3.

These systems are remarkably complex, even in the case N = 3, which already possesses fully chaotic dynamics [1]. A relatively simple sub-problem is to describe the *central configurations*, which with appropriate initial conditions give rise to relative equilibria in the planar case, and self-similar total collapse orbits in any dimension. A central configuration is defined by each particle being accelerated towards the center of mass with a magnitude proportional to its distance from the center:

$$\lambda(q_{i;j} - q_{C,j}) = \ddot{q}_{i;j} = \frac{1}{m_i} \frac{\partial U}{\partial q_{i;j}} = \sum_{k \neq j} \frac{m_j(q_{i;j} - q_{i;j})}{r_{i,k}^A}$$

We present some examples in this context of how considering the more general case of A > 2 can perhaps shed new light on the Newtonian problem (A = 2).

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# A High-Order Solver for the Scattering of Elastic Waves from Periodically Rough Rigid Surfaces

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We consider the elastic scattering of a time-harmonic plane wave from a rigid surface with periodic roughness. Our approach is based on a Helmholtz decomposition of the displacement function, which allows us to formulate the scattered field in terms of single layer acoustic potentials. Enforcing the usual boundary conditions on the rigid interface leads to coupled system of surface integral equations. Our numerical algorithm to solve the integral equations is based on the concurrent use of Floquet and Chebyshev expansions together with a specialized quadrature method we have developed for this problem. We demonstrate the rapid convergence of our algorithm to double precision accuracies for classically difficult cases where the peak-to-trough distance of the surface is many wavelengths deep.

#### An efficient quantum scheme for preserving the confidentiality of image data

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Image encryption is of vital importance in the gigantic and still developing domain of media transmission through public channels of any types. In this paper, a computationally-efficient quantum RGB-image encryption-decryption method is proposed based on BRQI (Bitplanes Representation of Quantum Images). To enhance the security efficiently, initially, a based bitplanes permutation scrambling method is used to turn the meaningful original image into a meaningless one by using some simple quantum operations. Afterwards, based on a key image, the encryption procedure is implemented, by which the generated encrypted image is capable of transmitting through public channels reliably. Experimental results comprising of Histogram diagram, Entropy rate and Correlation Coefficient of adjacent pixels analyzed in MATLAB environment show a good performance, proving that the proposed method is much more secure than the previous ones currently found in the literature. Moreover, regarding time complexity, the introduced method is able to be performed far better than its digital counterpart.

Key Words: Image encryption, quantum image encryption, quantum image decryp-

tion

# On one and two dimensional Cellular automata models and statistical wealth condensation: Conditions to generate a wealth-like distribution

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Cellular automata models are space-time-like discrete/continuous, deterministic/probabilistic dynamical systems, whose evolution is determined by local interactions. CA were firstly proposed by von Neumann and S. Ulam to understand the biological mechanisms of self-reproduction [1, 2]. These models are applied with success to model complex phenomena in physical, chemical, economical and biological systems [3, 4, 5]. In this work, wealth dynamics and wealth distribution emergence is investigated by different, two states one-dimensional and two-dimensional Cellular Automata models. To achieve this in the simplest way, we proceed as follows: for the different Cellular Automata models used in this research, we make them evolve and then we interpret each state change of a cell as the event of an agent gaining a "monetary unit". In this way, a "wealth-alike distribution" is generated for each one of the different Cellular Automata analyzed.

We show that the "wealth-alike distribution" generated by Conway's Game of Life Cellular Automaton (GoL) [6] is compatible with the exponential/gamma distribution observed in real Economic Complex Systems for the low and medium classes of the population of a country or a society. Furthermore, GoL also reproduces the power law asymptotic behavior observed in real socioeconomic data, corresponding to the richest sector of a population. Analyses of Gini index generated by GoL are also performed and discussed. Analyses performed with other different one and two-dimensional Cellular Automata rules are presented and discussed.

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## Lowest Energy Collective Modes in the Adsorption and Absolute Value Circular Dichroism Spectra of Helical Gold Nanorods

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We calculate, using time-dependent density functional theory, adsorption and circular dichroism spectra for a series of small helical gold nanorod structures with width 0.6 nm and length increasing from 0.6 nm for Au24 to 1.7 nm for Au56. For a low-energy window, ranging from 1.7 to 4.1 eV, broadening the lines in the adsorption spectra results in a lowest energy collective mode which we identify as the plasmon resonance. As expected, the peak position of the plasmon resonance systematically red shifts as the length of the nanorod increases. We further show that broadening the lines in the absolute value circular dichroism spectra results in a lowest energy collective mode with a peak position that systematically red shifts as the length of the nanorod increases but over a much smaller range than that for the plasmon resonance.

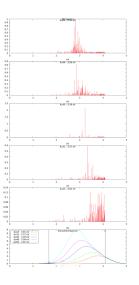


Figure 1: Raw and smoothed adsorption spectra.

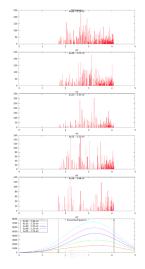


Figure 2: Raw and smoothed absolute value circular dichroism spectra.

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## Integrating discrete spatial simulation models and discrete global grid systems: a case study into wildfire modelling

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Study of forest fire modeling has received significant research attention during last decade [1-3] since forest fires have become one of the most critical natural hazards in recent years and they have direct impact on forests and consequently effect ecosystems. The main goal in wildfire modeling is to predict fire spread and intensity from easily measured variables [4] such as available fuel, weather variables such as temperature, evapotranspiration [5] and surface related parameters such as slope, elevation and aspect [6]. Cellular automaton (CA) is one of the approaches commonly used to study and predict natural phenomena such as gas, epidemic propagations, ecological modeling and urban studies [3]. In CA models, transaction rules between local neighbor cells around each cell are defined to predict each cell's status in specific time stamp [4][7]. Classic examples of CA include Conway's Game of Life; which illustrates how even simple rules can lead to complex spatial behaviors. The first applications of CA models in forest fire simulations was based on idealized heat transmission rules between burning and unburned neighbors under isotropic conditions [4]. The main challenge of using CA models to simulate complex natural processes is to define and parameterize the local transition rules governing the spatial dynamics of the process.

Discrete Global Grid Systems (DGGS) are of increasing interest as a new spatial data structure for the digital earth framework. DGGS are derived from a hierarchical multiresolution tessellation of the earth [8-9]. These tessellations are indexed with an indexing scheme that enables identification of spatial neighbors and parent-child relationships. Having a unique data structure to manage different data types in an integrated data structure and running models in large scale is one of the main goals of advent of DGG systems [10]. These systems are able to cover large scales and facilitate big spatial data management.

In this paper, we implemented a CA model within an DGGS data model. The cells in CA models could be square, hexagons and other shapes [4-5]. Hexagonal shaped cells have unique features such as equal distance between central cell and its neighbors and also having 6 main neighbors comparing to square grids could lead to more accurate results In CA models. A set of environmental parameters including weather data parameters, topological parameters and potential fuel parameters were used to simulate a large wildfire that took place in Fort McMurrey, Alberta in 2014. The input data were obtained primarily remote sensing data sources converted into the DGGS data structure. The gridding system which is used in this study is a hexagonal aperture 3 grid. For the initial step in CA modeling MODIS active fire product was used and in each time step of model total weights of each neighbor around each cell were calculated and based on this weight the next cell which has more potential of fire spread is selected. In each time step the previous fully burned cells were used as fire source. Results of our relatively simple CA modelling framework were compared to the Prometheus fire growth modelling tool widely used in Canadian fire management. We show that CA models can be implemented as decision support tools within a big data GIS system and conclude with a discussion of future research directions for spatially explicit modelling within a DGGS data model.

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## Agendas in Legislative Decision-Making

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Despite the wide range of agendas used in legislative decision-making, the literature has focused almost exclusively on two formats: Euro-Latin and Anglo-American agendas. To address the gap that this has left in our understanding of the legislative process, I first identify two structural features, history-independence and persistence, that are common among agendas used in legislative settings. I then characterize the social choice functions implemented by sophisticated voting (Ref. [1]) on agendas with these features. The result clarifies the connection between the structure of legislative agendas and the policies that they implement, thereby extending our understanding of legislative voting well beyond Euro-Latin and Anglo-American agendas.

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### **Collatz Approximation Semigroups**

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We apply computational Krohn-Rhodes theory to understand finite discrete dynamical systems approximating the Collatz function f on the positive integers. Mapping  $\mathbb{N}^+$  to itself by f(n) = 3n + 1 for n odd but f(n) = n/2for n even, the only known attractor cycle is (1,4,2). The long-standing Collatz conjecture asserts that, in this transformation semigroup  $C_1(\mathbb{N}^+) = (\mathbb{N}^+, \langle f \rangle)$ , all numbers eventually enter this cycle (e.g., [1]). That is, the conjecture says there are no other cycles and every trajectory is bounded. The related two-generator Collatz transformation semigroup  $C_2(\mathbb{N}^+) = (\mathbb{N}^+, \langle g, h \rangle)$  is obtained from two maps on  $\mathbb{N}^+$  by 'splitting' f into two functions: h(n) = 3n + 1 for n odd, but h(n) = n for n even, and g(n) = n/2 for n even, but g(n) = n for n odd. The semigroup  $\langle f \rangle$  defines a discrete dynamical system on  $\mathbb{N}^+$ , as does the semigroup  $\langle g, h \rangle$ . Each positive integer has the same orbit under the action of  $\langle g, h \rangle$  as under that of  $\langle f \rangle$ , even though the f cannot be written as a composition of g and h. Thus the Collatz conjecture holds if and only if it holds for this two-generated discrete dynamical system.

The monogenic Collatz approximation transformation semigroup  $C_1(N)$  on  $[N] = \{0, ..., N-1\}$  is obtained by taking the result of f modulo N. By taking the values of g and of h modulo N, one obtains a two-generated Collatz approximation semigroup  $C_2(N)$  on [N]. To gain insight into the Collatz problem, we make a computational and mathematical study of these finite one-and two-generated discrete dynamical systems approximating  $\langle f \rangle$  and  $\langle g, h \rangle$  acting on integer residues modulo N. In particular, we study the algebraic structure of these Collatz approximation semigroups using the methods of computational Krohn-Rhodes decomposition theory [2, 3, 4], including their idempotents, image sets, natural subsystems (permutation subgroups), and their holonomy decompositions. We consider the asymptotic behaviour of these characteristics as N approaches infinity, and seek to relate these to the properties of idempotents in topological semigroups extending the infinite discrete-event dynamical systems  $C_1(\mathbb{N}^+)$  and  $C_2(\mathbb{N}^+)$  using compactification constructions [5].

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### Stochastic modelling for population of Culex mosquitoes with temperature

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The impact of climate change on mosquito distribution and human health have attracted much attention in recent years and it is widely expected to significantly affect the spread, intensity and distribution of mosquitoborne diseases. Linking global and regional climate models with mathematical models of mosquito population dynamics provides a valuable tool towards improving and quantifying our understanding of how future climate change may affect the distribution of vector mosquito population. In this talk I will focus on using stochastic methods to model the dynamics of mosquito population with stochastic climatic factors. I will present some basic properties of the stochastic models and simulations to explore the variations of mosquito population under different weather patterns.

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### **State-dependent Model for Default Rate**

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Risk-weight function is a most popular formula for banking regulations to calculate the amount of backup deposit that banks need to hold in order to bear extraordinary losses. The model behinds the formula is introduced by Vasicek in 2002. In that paper, there are several intuitive appeal assumptions which are oversimplified. The most unrealistic assumption made by Vasicek is that correlations among each underlying exposure do not depend on the overall market environment. Dr. Adam Metzler has developed generalized version of the Vasicek model to release this assumption in 2017 which is called state-depend model. The model includes a parameter to allow the market correlation changes in a systemic way base on the overall economic level. We apply the EM algorithm that produce consistent estimates of the model parameters proposed by Dr. Adam Metzler. We also explore some properties of the model. The model involves a independence assumption that it assumes the default rate for each time is independent with each other. But according to the plots of the real historical data, that assumption is obviously violated. In order to relax the independent assumption, we bring a dependence structure to the model with respect to time by using the time series to model the so-call systematic risk factor M. We demonstrate that the changing of the market correlation has a huge impact on regulatory capital calculation.

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## **Sharp Fronts for the SQG Equation**

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Temperature discontinuities in the Surface Quasi-Geostrophic (SQG) equations support surface waves. For fronts that are described as a graph, the contour dynamics equation is a nonlocal quasi-linear equation with logarithmic dispersion. With smallness and smoothness assumptions on the initial data, solutions exist and are global. Numerical studies suggest the possibility of finite-time blow-up of solutions. For two SQG fronts the contour dynamics equations form a system with more complicated dispersion relations as well as quadratic nonlinearities. Based on a numerical simulation, spike-like singularities could form as a result of the extra Bessel-function dispersive term and the quadratic nonlinearities.

### Spatially Periodic Solutions of the Nonisentropic Compressible Euler Equations

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Glimm and Lax (1970) proved that small, spatially periodic solutions of the isentropic compressible Euler equations in one space dimension form shocks and decay like  $t^{-1}$  as time  $t \to \infty$ . Weakly nonlinear asymptotics indicates that much more complicated long-time dynamics may occur for small, spatially periodic solutions of the nonisentropic compressible Euler equations as a result of the resonant reflection of the left and right moving sound waves off an entropy wave [1]. This reflection leads to temporal oscillations in the sound waves, which can delay the formation of shocks or greatly weaken shocks after they form, raising the possibility that there are solutions which do not decay to zero as  $t \to \infty$ . We will review some of these asymptotic solutions and describe some recent work with Evan Smothers on the resonant reflection of very weak sound waves off a sawtooth entropy wave, which leads to particularly complex nonlinear dynamics [2].

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### Global Asymptotic Stability and Periodic Solutions in Cyclic Differential Delay Systems

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Systems of scalar differential delay equations of the form

$$x_i'(t) = -\lambda_i x_i(t) + \sum_{j=1}^n w_{ij} f_i(x_j(t - \tau_{ij})), \qquad i = 1, 2, \dots, n,$$
(1)

appear as mathematical models of numerous real world phenomena in neural networks, mathematical biology and physiology, economics and life sciences. See monographs [1, 2, 3, 4] for specific models, further applicability, and recent advances in theoretical and applied aspects. Such systems exhibit rich dynamical behavior including global asymptotic stability of equilibria, existence and stability of periodic solutions, instability, bifurcation, and complex/chaotic solutions among others.

We study a particular type of systems (1) when it has a cyclic structure, sign conditions on the nonlinearities involved, and the overall negative feedback. For the low dimensional cases n = 3, n = 2, and n = 1 we discuss some known results, derive several new results and propose a conjecture for the case of general dimension n.

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## **Oscillations and Periodic Solutions in a Two-Dimensional Differential Delay Model**

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We consider a system of two-dimensional differential equations with delays of the form

$$x'(t) = -\alpha x(t) + f(x(t), y(t), x(t-\tau), y(t-\sigma)), \quad y'(t) = -\beta y(t) + g(x(t), y(t), x(t-\tau), y(t-\sigma)), \quad (1)$$

where nonlinearities *f* and *g* are continuous real-valued functions, decay rates  $\alpha$ ,  $\beta$  are positive, and delays  $\tau$ ,  $\sigma$  are non-negative with  $\tau + \sigma > 0$ .

Sufficient conditions for the existence of periodic solutions in system (1) are established. The nonlinearities f and g are further assumed to satisfy either positive or negative feedback condition with the overall negative feedback in the system. The stability of the unique equilibrium and oscillation of all solutions about it are studied and derived in terms of the characteristic equation of the linearized system. The instability of the equilibrium together with a one-sided boundedness of either f or g lead to the existence of periodic solutions. The analysis of system (1) uses some of the results established for higher order differential delay equations [2, 3].

Systems of type (1) appear in various applications in engineering and natural sciences, in particular in mathematical biology and physiology as models of circadian rhythm generator [5] and glucose-insulin regulation models in humans[1, 4]

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## Finite-dimensional representation for infinite-dimensional dynamical system of nonlinear Klein-Gordon equations

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Nonlinear Klein-Gordon equations are studied in terms of the infinite-dimensional dynamical systems. Much attention is paid to the  $\varphi^{\alpha}$  -field theory type fractional power interactions ( $\alpha$ : fractional number). From a physical point of view, the fractional power is practical to incorporate the surface effect or finite-size effect to quantum many-body dynamics [1]. In this talk, based on our original precise-numeral scheme using the Fourier spectral method [2], a finite-dimensional representation method for infinite-dimensional dynamical systems is proposed. Such a precise scheme is necessary to deal with conservative wave propagation such as solitary wave propagation [3,4]. It enables us to analyze the detailed time evolution of infinite-dimensional dynamical systems. In conclusion a mathematical tool to investigate the breaking mechanism of conservation laws, as well as the symmetry-breaking induced by the initial-value sensitivity is newly provided. For a better understanding of finite-dimensional representation for infinite-dimensional dynamical system some comparison of different models are demonstrated by the computational graphic.

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## Optimal Control of a Vaccinating Game toward Increasing Overall Coverage

Monica G. Cojocaru and Ahmed S. Jaber

### Abstract

In this paper, we study an asymmetric game that characterizes the intentions of players to adopt a vaccine. The game describes a decision-making process of two players differentiated by income level and perceived treatment cost, who consider vaccination against an infectious disease. The process is a noncooperative game since their vaccination decision has a direct impact on vaccine coverage in the population. We introduce a replicator dynamics (RD) to investigate the players' optimal strategy selections over time. The dynamics reveal the longterm stability of the unique Nash-Pareto equilibrium strategy of this game, which is an extension of the notion of an evolutionarily stable strategy pair for asymmetric games. This Nash-Pareto pair is dependent on perceived costs to each player type, on perceived loss upon getting infected, and on the probability of getting infected from an infected person.

Last but not least, we introduce a payoff parameter that plays the role of cost-incentive towards vaccination. We use an optimal control problem associated with the RD system to show that the Nash-Pareto pair can be controlled to evolve towards vaccination strategies that lead to a higher overall expected vaccine coverage.

### **Controlling infection spread in a predator-prey system**

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#### Abstract

In this paper, we introduce an optimal control to two adjustments of the predator-prey system to model infectious disease of kind SIS or SIR. The proposed control parameter is considered as a preventive treatment provided to the susceptible prey compartment only. The infection in the predator population declined after reformulating the original system to an optimal control problem with necessary conditions. Moreover, a numerical method is implemented to solve the control problem and find the optimal solution. The preventive treatment is introduced into an existing predator-prey model from the work in [1]. We propose a susceptible-infected-susceptible-vaccinated (SISV) model and a susceptible-infected-recovered-vaccinated (SIRV) model. We analyzed these models as control problems initially proposed by the use of the steepest descent method to compute a numerical solution.

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### Learn-ability of Coordinate systems for Markov Processes

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Many interesting domains of problems can be expressed as finite state automata which have a representation as semigroups. From the Krohn-Rhodes theorem [2] its known that such semigroups can be decomposed into a cascade of elementary components, the inspection of which can lead to insights on the fundamental behaviours of the system as well as solutions to problems represented. For example Rubik's Cubes can be solved by "killing by layers" when a coordinate for the arrangement of the cube is provided.

Another hugely successful technique for solving a broad class of problems is deep learning. Deep learning generally makes very few assumptions about the structure of a problem an instead tries to learn relevant structures through training with lots of data. Although these two techniques seem somewhat orthogonal, there is potential for the strengths of both to be combined. It is also well known that how a problem is represented to a artificial neural network can have a huge impact on the performance and capabilities [3]. So as an example of how combining techniques might be beneficial, consider any two arrangements of a Rubik's cube, the shortest set of moves to transform from one arrangement to another might not be through the solved state. So its possible that using the coordinates provided by a semigroup decomposition as the representation of a problem, a deep learning solution will be able to more efficiently learn a solution that would be unnatural of difficult to find by analytical methods alone.

This presentation will cover recently completed preliminary investigations into the relative hardness of learning the transition model of a simple class of finite state problems using deep learning when using various types of coordinate inputs. In particular, arbitrary state labelling and holonomy decompositions [1] were used in an attempt to see if the latter representation provides any advantage to the deep learning model in solving the problem. The results of this inquiry showed that there does appear to be some interesting differences in learning behaviour depending on the coordinates used but for most measures the changes are slight and effects from changes in architecture necessary to accommodate the different coordinates forms could not be eliminated. However interestingly there does seem to be some effect when it comes to the ability to generalize to portions of the transition model held out from the training set. The data suggests that using holonomy coordinates might allow for a less "entangled" network which in future work I intend to explore if this property might lead to more interpretable networks.

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### **Fire Mediates Bark Beetle Outbreaks in Serotinous Forests**

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Bark beetle outbreaks and forest fires have imposed severe ecological damage and caused billions of dollars in lost resources in recent decades. The impact of such combined disturbances is projected to become more severe, especially as climate change takes its toll on forest ecosystems in the coming years. Here, we investigate the impact of multiple disturbances in a demographically heterogeneous tree population, using an age-structured difference equation model of bark beetle outbreaks and forest fires. We identify four distinct dynamical regimes for beetle and fire dynamics. The model predicts that fire helps dampen beetle outbreaks not only by removing host trees but also by altering the demographic structure of forest stands. Furthermore, we identify the optimal parameters for a stand thinning protocol that reduces the population size of the largest few juvenile classes by a small percentage in order to significantly reduce beetle-induced tree mortality and increase mature tree populations. Our research demonstrates one approach to capturing compound disturbances in a mathematical model. Such approaches will help us anticipate how forests might respond to upcoming changes in environmental regimes.

## **Exploring Tetris as a Transformation Semigroup**

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Tetris is a popular puzzle video game, invented in 1989. We formulate two versions of the game as a transformation semigroup and use this formulation to view the game through the lens of Krohn-Rhodes theory. In a variation of the game upon which it restarts if the player loses, we find permutation group structures, including  $S_5$ . This implies, at least in a simple case, that iterated Tetris is finitarily computationally universal.

# Travelling wave solutions, bifurcation analysis and conservation laws of reso-nance nonlinear Shrodinger's equation with Kerr law nonlinearity

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In this paper, travelling wave solutions of the resonant nonlinear Shrödinger's equation (R-NLSE) with Kerr law non-linearity are computed by using the equivalent form of  $exp(-\phi(\xi))$  method and bifurcation technique. Graphical representations of some solutions are given with different values of parameters to depict their propagation. It is observed that obtained solutions are blow-up, anti-peakon and super-nonlinear periodic solutions in nature. Further, bifurcation technique has been practiced for the considered equation. Four phase portraits are observed and classified with respect to the parameters of the equation. Moreover, a set of non-trivial and first-order conservation laws are computed by using different techniques.

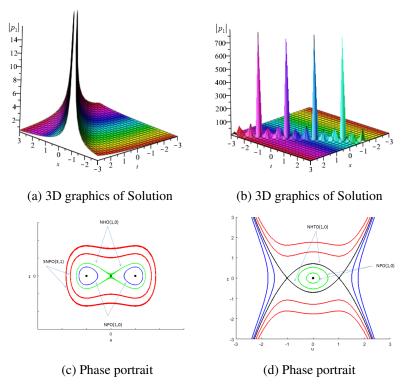


Figure 1

### Sampled-data $H_{\infty}$ filtering of a class of distributed parameter systems

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Distributed parameter systems (DPSs) have been receiving considerable enthusiastic attention due to its widely applications in heat transfer, wave propagation, chemical reactors, and traffic flow, etc. In recent decades, great progress has been made in the analysis and control of finite-sampling dimensional systems. However, few available results are developed to deal with the sampled-data control problem of DPSs with infinite dimensional characteristic. To enrich theoretical knowledge on infinite dimensional systems with external disturbance, much attention has been attracted on the filtering problem of DPSs, and some methods and theoretical results have been provided by the authors in [1][2][3].

This paper studies the  $H_{\infty}$  filtering problem of a class of DPSs with external disturbance. To compensate the effect of external disturbance, a filter with a sampled input is designed for the distributed parameter system (DPS). The stable conditions of the filter error system is derived to ensure that the filter can effectively observe the state of DPS, which is in terms of linear matrix inequalities by using the extended Jensens' inequality and Wirtingers' inequality techniques. Furthermore, the filter gain is given in specifically form.

The dynamic of the distributed parameter system is described as follows

$$w_t(x,t) = w_{xx}(x,t) + aw(x,t) + \delta(x,t), \quad t > 0, \quad x \in [0,l], w(0,t) = 0, \quad w(l,t) = 0, \quad w(x,0) = 0,$$
(1)

where  $w(x,t) \in R$  is the state, and  $\delta(x,t)$  is the external disturbance. Divide the domain [0, l] into N subdomains  $\Omega_i$  with a sensor placed in each  $\Omega_i$  providing the measurements

$$y_i(t) = c_i w(x,t) + d_i v(t), \quad i = 1, \cdots, N.$$
 (2)

where  $y_i(t)$  is the measurement outputs,  $c_i, d_i$  are two constants, and  $v(t) \in L^2(0, \infty)$  is the measurement noise signal. In the following, we introduce a filter for the distributed parameter system (1)

$$\hat{w}_{t}(x,t) = \hat{w}_{xx}(x,t) + a\hat{w}(x,t) + L\sum_{i=1}^{N} \chi_{i}(x) \left[ y_{i}(t) - c_{i}\hat{w}(x,t) \right], 
\hat{w}(0,t) = 0, \quad \hat{w}(l,t) = 0, \quad \hat{w}(x,0) = 0,$$
(3)

with the injection gain *L* and characteristic functions  $\chi_i(x) = \begin{cases} 1, & x \in \Omega_i, \\ 0, & x \notin \Omega_i \end{cases}$  i = 1, ..., N.

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### **Two-Phase Case-Control Study on Rare Event**

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Population health research platforms such as the Canadian Partnership for Tomorrow Project (CPTP) collect baseline information on participants and follow them forward in time to observed the development of disease. When analyzing the disease based on a large cohort, study designs such as a two-phase study and case-control cohort study can improve the progress with power and efficience. In a two-phase study, responses and Phase-I indirect covariates of the entire cohort are recorded, from which a subset will be represented for measuring additional variates of direct interest. In the meanwhile, a case-control control method acknowledges the presense of diseases during follow-up as the cases and samples case-control matchings to estimate impact of variables. However, in the case of some rare genetic disease, both chances of developing such disease and carrying the latent genome are unfortunately critical. With limited research budget and source, the call of exhibiting a powerful and efficient test design is put on board. Here, the proposed study will discuss the issues of the existing two-phase case-control cohort study on assessing rare events and exhibit a preferable study design.

Keys: two-phase study, case-control cohort, Cox Proportional Hazards Model, stratified designs

### A Resource Allocation Approach to Studying the Rules and resources

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Based on the knowledge and experience of the author from solving optimization and resource allocation problems in engineering, two principles are proposed in this paper. The first principle states that any rule, that exists in the physical world or can be considered mathematically, is defined or developed in relation to a resource allocation problem. The second principle states that any resource allocation problem indicates two types of limitations: (1) the limited resources and capabilities available to define or set the rules of resource allocation on one hand, and (2) the limited availability of the resources that are manipulated by resource allocation rules on the other hand. These two limitations on setting and defining the rules, and the avail-ability of resources which are manipulated by the rules can also be combined. These principles are explained and studied through several examples in different areas including mathematics, engineering and physics. Specifically, and interestingly, in natural sciences and physics, the principles conclude that the universe is defined and is running on limited resources.

### Mapping of Artificial neural networks and Brain health studies

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Mapping the brain provides valuable information about brain health. Also, artificial neural networks have been used in modelling the brain. While there is still a long way to successfully model the brain on computers, there has been continuous progress in modelling minicolumns which are segments of the brain that process the information as assumed in multilayer neural networks. In this paper, mapping input and output receptors of neural networks were studied. Mapping is used to study the effect of different damaged locations and levels in the neural network and to identify the characteristics of the damage. The results are then used to draw some conclusions regarding how neural networks and their mapping might be used in brain disease and health studies. The applied damages to the neural networks are similar to the lesions in the natural brain. The mapping of neural networks shows the sensitivity of the output nodes to input changes. This sensitivity analysis is used to identify the importance of each output node from the view of the input nodes. The representation is similar to maps of the natural brain.

## New Quota-based Apportionment Methods: The Allocation of Delegates in the Republican Presidential Primary

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We survey seven new, or at least previously unstudied, quota-based apportionment methods used by the Republican Party in their 2012 and 2016 state presidential primaries. After comparing the apportionment methods for three candidates using simplicial geometry, we evaluate how they differ in bias toward the top and bottom votegetting candidates. We also compare the methods to how they distinguish among candidates in close elections. We use the bias comparisons to discuss which methods should be used at different junctures in the primary season. We argue that states holding early primaries should select methods to build consensus of the party platform and that states holding late primaries should select methods that consolidate support for a top vote-getting candidate as momentum builds to the national convention. We compare our analysis to a timeline of the apportionment methods used by states in the 2012 and 2016 primaries. Finally, we discuss the susceptibility of the apportionment methods to different paradoxes.

### Integral points on continued fraction varieties

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It is well-known that the continued fraction expansion of a quadratic irrational is eventually periodic. In this talk we will discuss continued fractions of quadratic irrationals from a geometric point of view, describing affine varieties  $V_{k,n}(\alpha)$  that parametrize continued fractions associated to  $\sqrt{\alpha}$  in which an initial segment of length *k* is followed by a periodic part of length *n*.

We are particularly interested in the integral points on these varieties. When *n* is small, we can show that the integral points on  $V_{k,n}$  are not potentially dense when  $\alpha$  belongs to a number field. When *k* is small, the opposite appears to be true, and we can prove it in some cases. In small dimensions we study some of the intermediate cases by exhibiting compactifications by smooth normal crossings divisors and describing the log Iitaka fibrations explicitly.

## Structural Invertibility and Optimal Sensor Node Placement for Error and Input Reconstruction in Dynamic Systems

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A fundamental goal of science and engineering is to understand, predict or control complex dynamic systems, be they spreading infectious diseases, ecological networks, biochemical reactions, vehicles ore pace makers. ODE systems are routinely used for that purpose. However, our knowledge about most real world systems is limited and the system might be perturbed by external influences beyond our control. Reconstructing such unknown inputs from measurements is an important goal in order to observe the state of the system and to predict its future behaviour or to diagnose errors or attacks.

If the inputs can be reconstructed from measurements, we call such a system invertible. We present, how invertibility is related to the intrinsic network structure of the system. We show, that homogeneous networks undergo a transition from non-invertible to invertible (see Fig. 1(a)). We also found, that many real systems have a tendency to mask the inputs received. Therefore, invertibility requires a careful selection of outputs which need to be monitored by measurement devices. Importantly, we present a simple yet efficient sensor node placement algorithm to achieve invertibility of complex dynamic systems with a minimum of measurements (see Fig. 1(b,c)). These results are useful for the development of more realistic mathematical models, for the design of synthetic systems, and for the diagnosis of error or attacks with a minimum set of sensors.

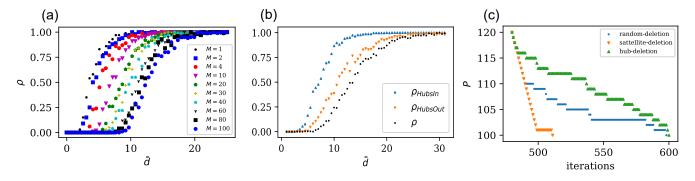


Figure 1: (a) The probability  $\rho$ , that a homogeneous network with average degree  $\overline{d}$  and M in- and outputs is invertible. For inhomogeneous (e.g. scale-free) networks the transition zone stretches over a larger area and they tend to have a lesser chance to be invertible. (b) In a scale-free network, the existence of hubs diminish the invertibility ( $\rho$ ). By preferential selection of hubs as output nodes ( $\rho_{HubsOut}$ ) or as input nodes ( $\rho_{HubsIn}$ ) invertibility can be increased significantly. (c) Three versions of a greedy output node selection applied to an exemplary network with randomly distributed inputs. Starting with a maximum output set, outputs are deleted until a minimum set of (in this example) 100 outputs is reached. As a consequence of (b), the sattelite-deletion reaches the optimum with the fewest number of iterations.

## Power-law distributions of high-incomers and formation of exclusive residential districts

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This paper discusses the relations of the spatial distribution of the number of highincomers living in each town in Japan and their total income totaled for each town, and propose a theoretical model of formation of exclusive residential districts.

Analyzing the database of high-income taxpayers in Japan, Kaizoji [1] found the following empirical evidence:

- (i) The complementary cumulative probability distribution functions of the number of high-incomers and the total income of high-incomers totaled for each of the towns follow a power-law distribution with an exponent which is close to 2.
- (ii) The number of high-incomers is positively correlated with the total income of high-incomers. Therefore, an exponent of the power-law distribution of the total income can be obtained from as a function of an exponent of the power-law distribution of the number of high-incomers, and
- (iii) the structure of the number of high-incomers and the total income of highincomers for each of the towns in Japan is very robust.

These empirical findings give light on that high-incomers tend to center on a small number of towns, and a large majority of high-incomer continues being a high-income and continues living in the same town. These empirical results help account for how the so-called high-class residential streets are formed by a small number of towns.

The empirical findings show that the total amount of income earned by high-incomers is largely determined by the number of high-incomers, and therefore suggests that in order, we need to understand a mechanism of generating a power-law distribution of the number of high-incomers as well as a power-law for income.

This paper aims to get a theoretically understanding of the buildup of high-class residential streets. Applying the mathematical model proposed by Irie and Tokita (2012), we propose a model to indicate that the power-law distribution of high-incomers can be derived from a positive relationship between the number of high-incomers and the total income of high-incomers.

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### Identification of communities in complex networks using hypergraph modularity

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Despite the fact that many important problems (including clustering) can be described using hypergraphs, theoretical foundations as well as practical algorithms using hypergraphs are not well developed yet [1]. As a result, researchers and practitioners are often forced to use a simplified approaches for investigating hypergraphs, such as creating the 2-section graph of a hypergraph of interest [2] or to restrict their study to *d-uniform* hypergraphs [3]. By using this methods we might lose some information about hipergraph's edges, which in some cases might have a profound impact on the obtained results.

In this talk we propose how hypergraph modularity function can be defined and how it can be used for identification of communities in complex networks. In order to define it properly, we generalize the Chung-Lu random model [4] for graphs to hypergraphs.

We present application examples using real-life data. The code is based on Julia programming language<sup>1</sup>, utilizing its many advantages. Julia allow the code to have around 4 times less lines (compared to C++ or Java) while maintaining similar execution speed and has significantly steeper learning curve, because of its syntax similar to popular interpreted, high-level programming languages such as Python or R. All computations are performed using SimpleHypergraphs.jl<sup>2</sup> open source library.

The project is partially financed by the Polish National Agency for Academic Exchange.

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<sup>&</sup>lt;sup>1</sup>https://julialang.org/

<sup>&</sup>lt;sup>2</sup>Avalaible at: https://github.com/pszufe/SimpleHypergraphs.jl/

### Mass-preserving solution-flux scheme for parabolic multi-interface problems

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Interface partial differential equations (PDE) are very important in science and engineering. A new masspreserving solution-flux scheme is proposed in this work for solving parabolic multi-interface problems. The whole domain is divided into sub-domains by interfaces with dis-continuous coefficients. The correction terms are proposed to the right hand sides of the solution-flux scheme at irregular points. It is calculated by given jumps of solution condition, flux condition and extrapolation strategies. We prove theoretically that our scheme satisfies mass conservation over the whole domain. The scheme is second order in space and first order in time. The accuracy and efficiency of our scheme are validated through several examples.

# $T - \psi$ formulation of an induction hardening model with a nonlinear constitutional relation for the magnetic induction field

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The induction hardening model is frequently used in industrial applications and described by Maxwell's equations coupled with a heat equation. Its analysis is quite complicated. In the case of linear constitutive relation, there are a lot of the published papers. But up to now there are very few works considering both a nonlinear constitutional relation.

In this talk, we study an induction hardening model consisting of the inductor with an alternating current, the workpiece and the surrounding air. The magnetic induction field is assumed a nonlinear constitutional relation and the electric conductivity is temperature-dependent. The source term in the heat equation is handled approximately by the truncated quadratic Joule heating term. The  $\mathbf{T} - \boldsymbol{\psi}$  method (called reduced magnetic scalar potential formulation) is to transform Maxwell's equations to vector-scalar potential formulations and to solve the potentials in the framework of the finite element method. We present the  $\mathbf{T} - \boldsymbol{\psi}$  formulation for this nonlinear coupled problem and discuss its solvability. First, we design a nonlinear time-discrete decoupled scheme, investigate existence and uniqueness of the approximate solution and derive some stability estimates. Then, we use Rothe's method to conclude convergence of subsequences of the approximate solution in appropriate function spaces. Next, we prove that the convergence limit is the weak solution of the continuous problem. Finally, we solve it by means of the  $\mathbf{T} - \boldsymbol{\psi}$  method and show some numerical simulations.

### Inference with Sparse Covariance and Precision Matrices

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Over the last 20 years, much effort has been put into estimation of covariance and precision matrices for high dimensional data. The high dimensional setting,  $n \ll p$ , requires additional structural assumptions due to the large number of parameters to be estimated. In the cited articles, we proposed a method for such estimation under the assumption of sparsity—i.e. most of the off-diagonal matrix entries are equal to zero. Similar to most other sparsity-based esitmation methods, we make use of a regularization parameter to enforce the level of sparsity in the resulting estimator. Unlike other estimators, our regularization parameter is interpretable; it is the false positive probability for incorrectly deciding that a matrix entry is non-zero when in truth it is zero. That is,

P(false positive) := P  $(\hat{\Sigma}_{i,i} \neq 0 \mid \Sigma_{i,i} = 0)$ .

In this talk, we will discuss three different inferential techniques making use of sparse covariance and precision estimators. The estimators and inferential tools can be found in the sparseMatEst package on CRAN.

The first is random design regression. In random design regression, we take the design matrix  $X \in \mathbb{R}^{n \times p}$  to be comprised of *n* iid rows with mean zero and covariance  $\Sigma$ . The standard least squares estimator relies on the matrix  $(X^tX)^{-1}$ , which does not exist when p > n. Instead, we replace  $(X^tX)^{-1}$  with a sparse estimator.

The second is linear and quadratic discriminant analysis. Similar to the random design regression setting, classifying data with LDA or QDA requires estimation of  $\Sigma^{-1}$ , the precision or inverse covariance matrix. Under the assumption of sparsity, we fit such a classifier and compare it with other high dimensional classification methods.

The third is clustering with Gaussian mixture models. Fitting an uncontrained Gaussian mixture to a data set requires many parameters to be estimated. While much work has been done on model based clustering and model selection for Gaussian mixtures, we make use of the sparse covariance estimators to adaptively determine the covariance structure in each cluster.

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### **Inverse Problem for a two-dimensional Fractional Parabolic Equation**

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We will consider a Samarskii-Ionkin type problem for two-dimensional fractional parabolic equation

$${}_{C}D^{\alpha}_{0t}u + \frac{\partial^{4}u}{\partial x^{4}} + \frac{\partial^{4}u}{\partial y^{4}} = f(x, y, t)$$

where  ${}_{C}D^{\alpha}_{0,t}u, \alpha \in (0,1]$  is the derivative of order  $\alpha$  in the sense of Caputo.

We investigate the solvability of a non-local problems in using the Fourier method of the separation of variables and study the completeness of the root functions of the corresponding spectral problems. Also, using the properties of biorthogonal systems, we study an inverse problem of identifying the source time independent function f in the spatial domain.

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## **Desaturation of Granular Materials in Conical Filtering Centrifuges**

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A model for steady-state continuous liquid extraction from a cake of wet granular material in a conical filtering centrifuge is presented (Fig 1.a) [1]. Unlike previous models [2], effects of capillary and adsorptive forces are taken into account by using the liquid retention curve and the hydraulic conductivity function. It is assumed that the cake thickness is divided into a constant number of layers,  $N_{layers}$ , with thickness,  $\Delta z^{layer}$ . These layers do not mix and they move without internal shear and at the same slip velocity. The differential equation describing desaturation of the cake when it moves from position r to  $r+\Delta r$  is derived based on the mass balance and the Darcy-Buckingham equations as follows:

$$\frac{\partial\theta}{\partial r'} = -\frac{1}{u_s^{drain}} \frac{\partial}{\partial z^{drain}} \left( K(h) \left( \frac{\partial h}{\partial z^{drain}} + \frac{\omega^2 (r' \sin \alpha - z^{drain} \cos \alpha) \cos \alpha}{g} \right) \right),\tag{1}$$

where: *h* is the pressure head,  $\theta$  is the volumetric liquid content,  $u_s^{drain}$  is the slip velocity of the cake along the screen (radial direction), *r'* is a radial coordinate between *r* to  $r+\Delta r$ ,  $z^{drain}$ : is a height coordinate along the thickness of the cake,  $\omega$  is the rotation speed,  $\alpha$ : is the cone angle, *g*: is the gravitational acceleration and *K* is the hydraulic conductivity. Equation (1) is non-linear and is solved in the interval:  $r \leq r' \leq r + \Delta r$  by assuming constant cake height and using the algorithm presented in the literature [3]. The coordinates where volumetric liquid content and pressure head solution are obtained correspond to the mid-height of the cake layers with thickness  $\Delta z^{layer}]_r$  (blue dot in Fig. 1.b). The cake layer thickness and slip velocity at  $r + \Delta r$ :  $\Delta z^{layer}]_{r+\Delta r}$ ,  $u_s]_{r+\Delta r}$  are updated using the volumetric liquid content obtained from the solution of equation (1), the solid phase mass balance equation -conservation of cake volumetric flow rate- and the stress balance equation at the cake – screen interface. Calculated volumetric liquid contents and pressure heads at mid-height positions of layers with thickness  $\Delta z^{layer}]_{r+\Delta r}$  at  $r + \Delta r$ . After modeling cake evolution in the step from *r* to  $r + \Delta r$ , both liquid and solid masses are conserved. The process is repeated sequentially for every radial step,  $\Delta r$ , between centrifuge inlet and outlet, by updating the velocity and the cake layers thickness. Thus, the evolution of the layers thickness, velocity and volumetric liquid content are predicted sequentially along the radial direction. Effects of number of layers and radial steps on the results are presented. The model can be used as a design tool for conical filtering centrifuges.

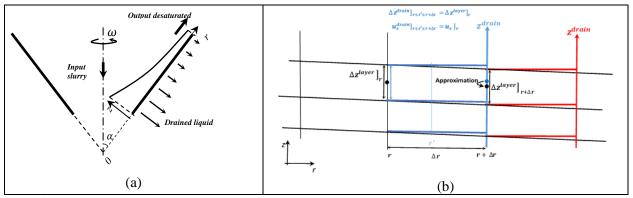


Figure 1: (a) Conical filtering centrifuge, (b) Discretization used for the solution of the desaturation equation.

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### Advances in Subgradient Computation for Nonsmooth Optimization

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Established optimization methods for smooth problems may fail entirely when applied to nonsmooth problems, since descent directions may no longer be described in terms of a single gradient. Instead, dedicated methods for nonsmooth optimization typically use subgradients to gather useful local sensitivity information; subgradients are essentially nonsmooth analogs of gradients. However, evaluating subgradients may be challenging in itself, particularly when the underlying system includes dynamic behaviour modeled using systems of differential equations, since subgradients obey weaker calculus rules than gradients.

This presentation describes several recent and new advances in subgradient evaluation for nonsmooth problems, including an efficient method (Ref. [1]) for computing subgradients automatically for composite nonsmooth functions, the first general method for subgradient computation for nonsmooth systems of parametric ordinary differential equations (Ref. [2]), and a new method for computing subgradients that is specialized for functions of two variables. These methods all make heavy use of techniques and concepts from algorithmic differentiation methods developed for smooth functions. In particular, the "branch-locking" method of Ref. [1] proceeds by temporarily replacing the underlying nonsmooth problem with a certain smooth variant, and then applying classical algorithmic differentiation to that variant. Implications and applications are discussed.

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### Existence and approximation of attractive points

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Takahashi and Takeuchi [1] introduced the idea of attractive points. Approximation of (common) attractive points has been done basically by classical iterative processes: Picard, Mann, Ishikawa iterative processes and their multistep variants. The author [2] introduced an iterative process called Picard-Mann iterative process. This iterative process got a good attention of researchers and had many generalizations. The author [3] has also introduced the ideas of common attractive points and further generalized mappings. Established were the existence of common attractive points and their approximation through a generalized version of the afore-mentioned Picard-Mann iterative process. Here we use a more recent iterative process to approximate attractive points of these mappings. Our three-step iterative process is defined as follows.

Let  $T : C \to C$  be a nonlinear mapping defined on a convex closed subset *C* of a Hilbert space *H*. Define the sequence  $\{x_n\}$  iteratively as follows.

$$\begin{cases} x_{n+1} = Ty_n, \\ y_n = T((1-\delta_n)z_n + \delta_n Tz_n), \\ z_n = T((1-\mu_n)x_n + \mu_n Tx_n), n \in \mathbb{N}. \end{cases}$$

This iterative process converges faster than above-mentioned classical iterative processes. We prove some existence as well as convergence results for attractive points of T using the above iterative process. We also give a comparison of attractive and fixed points. This will improve and generalize several results including those of Khan [3].

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# Simulating Elastic-like Polypeptides to Better Understand the Mechanical Properties of Materials

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Elastin-like polypeptides (ELP) are a class of biomaterials that are engineered to be used for different applications, especially as the replacement of natural tissues. Tuning their biochemical and biomechanical properties could affect their behaviours, such as elasticity, cell binding, and signaling, introducing a variety of potential applications for these types of materials. In this project, we use a mixture of different ELP proteins, in addition to ligands to mimic the experimental environment of the system. As a part of this project, we study the effect of pH (implicitly) on the interactions and the overall structure of the system. Here, we use the GROMACS package to run all-atom molecular dynamics simulations of our system. We study the effect of pH on the interactions between THPC ligand and different peptides in the ELP mixture. Our results provide more insight into the interactions in the system and elaborate effect of pH on the structures of the ELP, as reported in the experiments.

The Prevalence and Consequences of Ballot Truncation in Ranked-Choice Elections M. Kilgour<sup>1</sup>, J.-C. Grégoire<sup>2</sup>, A. Foley<sup>1</sup>

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In ranked-choice elections, voters vote by indicating their order of preference over the candidates. A ballot is truncated when the ordering is incomplete (this is called partial voting). Sometimes truncation is forced--voters are allowed to name only a limited number of candidates--but sometimes it is voluntary. During the counting process, a truncated ballot is exhausted when all of the candidates it names have been eliminated. Ballot exhaustion, and therefore ballot truncation, is a concern in single-winner elections when the margin of victory in the final stage is less than the number of exhausted ballots. This concern motivates our study.

We review evidence from actual single-winner ranked-choice elections and conclude that voluntary ballot truncation is very common. Moreover, it is difficult to explain strategically. To assess the significance of ballot truncation, we simulate ranked-choice elections with four, five, and six candidates, using both spatial and random models of voter preference. Does truncation change the probability that a Condorcet winner wins the election? Does the winner change as the amount of truncation increases? We find that even small amounts of truncation can alter the election outcome.

## Large Bound States in Schrödinger Equation with General Nonlinearities

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I will discuss recent progress in finding all ground states at large eigenvalue (chemical potential) parameter for the Schrödinger equation with general, attractive nonlinearities. The work is part of the project to find all coherent (bound) states of NLS by combining global bifurcation theory with finding all the limit points of coherent state branches at the boundary of the domain where the linearized operator is Fredholm. This particular talk focuses on the portion of the boundary where the eigenvalue parameter is infinity and builds upon the results previously obtained by the first author for the case of power nonlinearities.

## **Optimal Static Hedging With Quantile Regression**

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In this talk, I will present a model-independent approach to finding static hedges for general path-dependent options. In particular, I will discuss non-parametric methods of estimation of optimal static portfolios using quantile regression methods. Such an approach is possible due to an explicit representation of an optimal hedging option under general conditions, where the criterion for optimality is the expectation of the shortfall weighted by some loss function. I will focus on two aspects of the proposed framework: the rate of convergence of the estimated strategies to the optimal ones and the sensitivity of the hedging method to some assumptions about the dynamic of the underlying price process. The method will be illustrated with some applications to path-dependent options.

## A kernel-independent treecode based on barycentric Lagrange interpolation

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A kernel-independent treecode (KITC) is presented for fast summation of pairwise particle interactions. In general, treecodes replace the particle-particle interactions by particle-cluster interactions, and here we utilize barycentric Lagrange interpolation at Chebyshev points to compute well-separated particle-cluster interactions. The scheme requires only kernel evaluations and is suitable for non-oscillatory kernels. For a given level of accuracy, the treecode reduces the operation count for pairwise interactions from  $O(N^2)$  to  $O(N \log N)$ , where N is the number of particles in the system. The algorithm is demonstrated in serial and parallel simulations for systems of regularized Stokeslets and rotlets in 3D, and numerical results show the treecode performance in terms of error, CPU time, and memory overhead. The KITC is a relatively simple algorithm with low memory overhead, and this enables a straightforward efficient parallelization.

We look forward to welcoming you in Waterloo, Canada at the AMMCS Conference!

Figure 1: The AMMCS Conference is organized in cooperation with SIAM and AIMS.

## The NEU Meta-Algorithm for Geometric Learning

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We introduce a meta-algorithm, called non-Euclidean upgrading (NEU), which learns algorithm-specific geometries to improve the training and validation set performance of a wide class of learning algorithms. Our approach is based on iteratively performing local reconfigurations of the space in which the data lie. These reconfigurations build universal approximation and universal reconfiguration properties into the new algorithm being learned. This allows any set of features to be learned by the new algorithm to arbitrary precision. The training and validation set performance of NEU is investigated through implementations predicting the relationship between select stock prices as well as finding low-dimensional representations of the German Bond yield curve.

#### Nonlinear effects in designing environmentally-friendly lead-free piezocomposites

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Lead-free piezocomposites are emerging as prospective materials for scalable and sustainable sensing and harvesting of mechanical energy [1]. However, the efficient design of such composites requires an understanding of various physical processes that underlie the performance in addition to the linear piezoelectric response, which is the conventional measure of performance. Specifically, nonlocal and nonlinear effects could have significant size- and strain-dependent contributions to the overall piezoelectric response [2-4]. Here, we develop a non-linear electro-elastic finite-element-based model to account for electrostrictive and linear piezoelectric effects in BaTiO<sub>3</sub>-based lead free composites. The physical relations linking the stress  $\sigma_{ij}$ , strain  $\varepsilon_{ij}$ , electric field  $E_i$ , and electric flux  $D_i$ , are given by [2-4]

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} - e_{kij}E_k - \frac{1}{2}B_{klij}E_kE_l, D_i = \epsilon_{ij}E_j + e_{ijk}\varepsilon_{jk} + B_{ijkl}E_j\varepsilon_{kl}, \tag{1}$$

where  $c_{ijkl}$ ,  $e_{ijk}$ ,  $e_{ijk}$ ,  $e_{ijk}$ , and  $B_{ijkl}$  are the elastic, piezoelectric, permittivity, and electrostrictive coefficients respectively. These equations are further subject to force and charge balance laws and boundary conditions, which completely describe the system.

We present our findings related to the strain-dependent contributions of nonlinear electro-elastic response of the composite in terms of generation of electric flux and electric fields, which are both critical for energy harvesting applications. Further, we present the design of piezocomposites with nanomaterial-modified matrices, which have tailored elastic, dielectric, and electrostrictive properties, tuned to maximize the performance of the composites in the context of sensing and energy harvesting. In particular, we note that the contribution due to the nonlinear processes becomes significant at higher strains, where a considerable amount of electric flux is generated through such processes, in addition to the piezoelectric flux. The electric field distribution within the composite, however, is almost unaffected by the nonlinear processes. This shows that at larger strains, BaTiO<sub>3</sub>-based piezocomposites of the matrix using carbon-based nanomaterials. This work, therefore, paves way to refined models for piezocomposite design and provides novel options for optimizing the performance of such materials.

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# Breast Cancer Risk Prediction using Magnetic Resonance Imaging in Women of High Risk

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Breast cancer (BC) is a common malignancy of women arising in the epithelial cells of the ducts or lobules that compose the fibroglandular tissue (FGT) of the breast [1]. BC screening has been utilized for women since the middle of the 1980s and in a Pan-Canadian study of mammographic screening in 2014, screening lowered the mortality rate by 40% [2]. In 2011, the Ontario Breast Screening Program began a high risk screening group (HRSG), the first of its kind in Canada and possibly the world, to facilitate annual mammograms and breast Magnetic Resonance (MR) imaging for this group [3], due to the synergistic performance of combination screening. The inclusion criteria is based on genetic counseling using current risk assessment modeling tools. A critique of these models is their lack of non-genetic information, such as tissue characteristics observed in radiographic investigations [4]. Research initiatives to develop a more precise calculation of individual patient risk are being sought to begin discussing more personalized screening protocols.

At Sunnybrook Research Institute (SRI), breast MR data has been archived since the early 2000s, resulting in a curated data base of nearly 10,000 MR screening scans from over 2000 women. Our hypothesis is that MR imaging from the HRSG can be used to reveal an understanding of an individual patient's risk based on their tissue features. This entails the segmentation of breast tissues (FGT and fat) using a deep learning algorithm called a Unet [5]. This algorithm has given us an average dice similarity coefficient of  $0.94 \pm 0.05$  standard deviation for fat tissue and  $0.88 \pm 0.09$  for FGT when evaluating the 3-D volume of one breast. This automated method can now be used to calculate volumetric measures such as percent FGT (%FGT) and background parenchymal enhancement (%BPE).

Our further work will entail the development of a Tissue Texture Score (TTS) using deep learning features and image texture analysis. Unsupervised learning methods will be explored to simultaneously learn features and cluster groups using Deep Embedded Clustering [6], alongside a Siamese network [7] to quantifying breast asymmetry [8]. TTS, %FGT and %BPE can then be evaluated for statistical significance for predicting BC risk using logistic regression.

The outcomes of this research has the potential of give a greater understanding of BC risk from MR imaging, aid the health care system in allocating scarce financial resources, and assist in the detection and management of false positive reports.

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## Fuzzy Logic Model to Identify the Authenticity of Claim of Insurance

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The preventive avoidance of cancellation is a key problem facing insurance companies. A conversation with the client held prior to latter's decision to cancel a contract increases the likelihood of contract continuity. So companies are in need of reliable expert system that can help them to evaluate the risk of cancellation of the policies in future. With the help of fuzzy system it is possible to identify clients who may potentially cancel and take timely measure to safeguard the portfolio. Here a model is presented, which is designed by using fuzzy mathematics and expert system to provide indicative results on the risk of cancellation of the policies in future.

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# Stochastic self-assembly of HIV-1 Capsids using an extended Becker-Döring Model

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During the maturation of HIV-1 virions, various components come into play and include MA (matrix proteins), CA (capsid proteins), NC (nucleocapsid proteins) and RNA (ribonucleic acid). The CA plays an important role in the life cylcle of an HIV-1 virus. About 1000-1500 CA monomers are needed to build a typical cone-shaped capsid [5]. The self-assembly of HIV-1 will be modeled here using an extended Becker-Döring model, and the mean first assembly time to form a cone-shaped capsid will be determined.

The Becker-Döring model is one of the most popular models to describe aggregation and detachment in the self assembly of molecules.

$$C_r + C_s \stackrel{k_r^+}{\underset{k_{r+s}}{\rightleftharpoons}} C_{r+s} \tag{1}$$

Here,  $C_r$  are the concentrations of a cluster of size r, where r can be referred to as aggregation number and, r = 1, 2, 3.... The  $r^{th}$  forward reaction rate constant is  $k_r^+$ , and  $k_{r+s}^-$  is the  $(r+s)^{st}$  backward reaction rate constant. The Becker-Döring system (s=1) allows for clusters. We assume that the system follows the law of conservation of mass. We are using the model assuming that it is a chemical reaction. The exact solution for this ODE model is derived from mass action nucleation theory for spontaneous homogeneous self-assembly. The stochastic model for the Becker-Döring model based on the forward and backward master equation is derived, and used to find the mean first assembly time (MFAT). The corresponding set of chemical reactions for the model, that can be used to get appropriate stochastic trajectories for comparison with the corresponding ODE solution for this model will be derived. One of the limitations of the Becker-Döring model is extended here to include attachment and detachment of molecules of size two or more in a cluster(s=2,3,... in equation (1)), one at a time, with the help of a chemical master equation and stochastic approaches. The mean first assembly times of molecules of different sizes based on the extended Becker Döring Model will be determined scholastically.

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# Solving Inverse Problems for Elliptic Equations Using the Generalized Collage Theorem and Shannon Entropy

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Collage-based Inverse Problems can be viewed in terms of the approximation of a target element in a complete metric space by the fixed point of a contraction mapping [1]. These ideas have been extended to inverse problems for ordinary differential equations in recent papers [3-5]. Recently the Collage Theorem has been generalized to study inverse problems for partial differential equations [2,6-7].

In this talk, we show how the results obtained by the generalized collage theorem can be further improved by adding Shannon entropy to the minimization algorithm. A similar analysis was done for collage-based inverse problems in the case of ordinary differential equations in [8]. Numerical results show how the methods works practically.

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# Integral equation solution for two-dimensional simulations in nanoplasmonics; single layer vs multi-layer 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 paper, an integral-equations formulation is given for an infinitely periodic metal surface whose period d is on the nanometer scale. The metal is assumed to extend infinitely below this surface, while a dielectric material extends infinitely above the surface. In this paper, we also, offer to extend this achievement to a more challenging case; multilayer configurations. The new configuration will composed of a thin layer of noble metal (gold, silver, etc.) with depth larger than skin depth of the material, buried into different epoxies on top (glass/polymer substrate) and the bottom (liquid/water/blood). Some details of the numerical implementation and the results of a few numerical simulations and experimental comparisons are also given.

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## **Computer Modeling of Assembly of Non-convex Nanoparticles**

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Highly non-convexed nanoparticles have attracted the interest of the scientists[1], because they offer many possibilities for the fabrication of functional materials as a result of their ability to self assemble into unique structures driven by mechanisms absent in convex particles. These mechanisms include interlocking, entanglement, and interpenetration[2].

Star-shaped nanoparticles are a class of non-convexed nanoparticles. The "star"-shaped nanoparticles have found many applications. The sharp tips of gold nano-stars have been shown to enhance the electromagnetic field of surface-enhanced Raman scattering (SERS), an imaging technique used in the imaging of cancer tissues[3]. The same effect have also been utilized in photothermal therapy, a cancer treatment technique that irradiates the area of a cancerous tissue with an infrared laser matching the excitation wavelength of the nano-stars. The gold nano-stars convert the incoming light to heat, and focus the heat on its sharp tip to destroy the cancer cells [4].

Here we study the assembly mechanisms of star-shaped nanoparticles with atomistic modelling, where the shape of the nanoparticles is maintained with restraint. Using the multi-point shapes already obtained in our past molecular simulations, we have found several "metastable states" where the distance between two stars stay constant while the two stars rotate to find the minimum energy path for the assembly process to proceed.

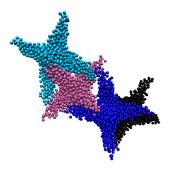


Figure 1: A snapshot of a four nanostar cluster.

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## Optimal Control of a Spatial Economic Growth Model with Physical Capital Accumulation and Pollution Diffusion

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We propose a new Ramsey-type model (see [7,9]) to study the dynamic evolution of physical capital and pollution over space and time (see [1-6,8]). The decision maker seeks to maximize his/her intertemporal utility, maximize the level of physical capital and minimize the level of pollution. We also propose a new algorithm to determine the optimal policy, and numerical simulations to show how the method works practically.

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## Derivatives on Fractals Generated by Iterated Function Systems and Their Application

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Many physical phenomena can be described by variational problems involving bilinear forms. Classical models and techniques to solve these kinds of problems rely on the assumption that a derivative or a gradient is defined and that the underlying domain is smooth. However, non-smooth structures appear frequently in physical phenomena creating "irregular" and "rough" objects. [1,4,6]

The notion of differentiability [3,9,10] on fractals [2,5,8,11] has been studied by many authors in the literature, mainly using approaches based on sequences of sets and measures approximating the fractal from inside or outside.

Based on a recent paper of the same authors [7] in which we study solutions of a variation of a classical integral equation (based on the Picard operator) in which Lebesgue measure is replaced by a self-similar measure  $\mu$ , this talk is about how to extend these results to the case of weak derivatives and variational problems involving bilinear forms on fractals.

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### **Decaying Aspects of Quantum States Under Noise**

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A central challenge in quantum information is the decay of quantum states toward mixture or equilibrium. This decay appears in decohering qubits, noisy transmissions, quantum memory, and most if not all available media that store and process quantum states. We model decay processes as continuous quantum Markov processes or discrete quantum channels. We quantify useful properties in resource theories, as distance to or fidelity with an undecayed or fully decayed state, or by special forms of relative entropy.

In previous works with a variety of collaborators [1, 2, 3], we used the mathematical techniques of complex interpolation, symmetric extendibility and transferred heat kernel estimates to bound various notions of communication capacity and decoherence times. In this talk we present a generalized framework to analytically estimate how different aspects of quantum states decay. These include resources like coherence and asymmetry, as well as criteria like Bell and positive partial transpose test violations. We define and estimate a channel's potential to preserve entropic resources, comparing to existing notions of a channel's ability to generate resources. We show that many quantum information estimates naturally generalize to a wide variety of settings and aspects.

In some cases there is a "breaking" point: a point at which the state has not fully decayed, but a discrete, useful property is no longer present. Examples include entanglement-breaking in channels and thresholds for scalable error correction. Breaking is a combined aspect of the desired property and the channel, and we begin to classify general criteria under which such a point appears. We bound allowable time between active error correction steps for various error models, and we estimate the maximum depth of noisy quantum circuits proposed as a near-term quantum computing paradigm [4].

MJ and NL are partially supported by NSF grant DMS 1800872.

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#### Symmetry and the Tradeoff Between Model Specificity and Effective Sample Size

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A common theme in modeling and machine learning for high-dimensional data is to distill relevant features from details and noise. Efficient models [1] also leave out some relevant variables and features, because the computational cost of inclusion outweighs the benefits. With finite data, this principle goes a step further: even relevant variables can increase a model's error, even without directly counting the computational cost.

We quantify this principle using ideas inspired by the study of symmetry in stochastic systems [2, 3] and quantum information theory [4]. Qualitatively and intuitively, a good model model is asymmetric to relevant features, and symmetric to irrelevant features. While the qualitative idea has existed before [5], we present quantitative bounds with applications to specific modeling approaches. For large sample size and sufficiently independent errors, an adaptation of information-theoretic typicality combined with the Khintchine and Rosenthal inequalities analytically estimates total error change from re-weighting training datapoints for a given test point according to an additional variable. For smaller sample sizes, direct computation is tractable without the typicality approach. Conditioned on relevant variables, optimal weighting maximizes entropy. In simple cases, we can calculate an effective sample size depending on the weighting in the process it uses to generate outputs from a given input. Intuitively, the more features a model includes, the fewer training points will be relevant to a given scenario.

We begin to link the conceptual intuition behind model sloppiness [6], information bottlenecks [7], information leverage [8], and dewdrop regression [9]. We explain why sometimes, even apparently relevant features are best ignored. While it is well known that model efficiency implies discarding some information to optimize computational cost, explicitly penalizing computational cost may not always be necessary. Optimal model construction should dynamically adjust the level of specificity according to the availability of specific training data.

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## Utilizing Bidirectional Encoder Representations from Transformers for Answer Selection Task

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The Bidirectional Encoder Representations from Transformers (BERT) [2] model has been found very effective in different Natural Language Processing (NLP) tasks recently. The BERT model is pre-trained on language modeling task and it can provide contextualized representations of each token in a sentence. Though the fine-tuned BERT model has provided state-of-the-art results in different NLP problems, to our knowledge it has not been evaluated for the answer selection task yet. In this work, we fine-tune the pre-trained BERT model (see Figure 1) for the answer selection task. In the task, a question is given along with some candidate answers. The goal then is to rank the candidate answers based on their similarity with the question. More specifically, we take the question  $X = x_1, x_2, ..., x_m$  and the candidate answer  $Y = y_1, y_2, ..., y_n$  as input to the BERT model. Then the sentences are combined together into a single sequence, separated by a special token [*SEP*]. The final hidden state *C* of the first token ([*CLS*]), which is the aggregate representation of the sequence, is used for classification. During fine-tuning, parameters are added for an additional classification layer *W*. All the parameters of the pre-trained BERT model along with *W* are fine-tuned jointly to maximize the probability of the correct label. The label probabilities  $P \in \mathbb{R}^K$ (where *K* is the total number of classifier labels) are calculated as follows:

$$P = softmax(CW^T) \tag{1}$$



Figure 1: Fine-tuning the BERT model: The tokens of question *X* and a candidate answer *Y* are combined together as input to the pre-trained BERT model. The parameters are then fine-tuned based on the classification output.

We evaluate the effectiveness of the fine-tuned BERT model on two different datasets, namely, the TREC-QA and the WikiQA. We observe new state-of-the-art results for the answer selection task in both datasets. In terms of Mean Average Precision (MAP) metric, the fine-tuned BERT model has an improvement of 6.18% in the TREC-QA and an improvement of 13.72% in the WikiQA datasets respectively over the state-of-the-art approaches [1].

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# **Investigating Model Improvement Using Fractional Differential Equations: An Inverse Approach**

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Mathematical modelling of real world phenomena via integer order differential equation (DE) models has been a popular topic of research for decades. A wide variety of articles have been written in this area and major advancements in model accuracy have been made. Some more recent research suggests that fractional order DEs may more efficiently and accurately model real world phenomena than their integer order counterparts. While the roots of fractional Calculus date back to the 1800's, its use in fractional order DEs is much more recent (see for instance, [1]). The development of solution techniques (both closed form and numerical) to fractional DEs have been proposed in a number of more recent articles. In this talk, we investigate improvements to integer order DE models for fitting experimental data using fractional DE models. Unknown parameter values, including the fractional order of the DE, are determined using a collage-coding inverse problem technique and results are compared and contrasted.

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#### Solving norm equations over function fields using compact representations

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Solving norm equations is a classical problem that has a long history in number theory. While there is a considerable body of research dedicated to them over number fields, norm equations over function fields are significantly less studied. The main algorithm for solving norm equations over function fields, due to Gaal and Pohst [1], requires representing units and performing exponentiation on them. The standard representation of a unit  $\alpha$  of the maximal order  $O_F$  of a function field F over the finite field  $F_q$  with respect to an integral basis  $\mathscr{B} = \{b_i \mid 1 \le i \le n\}$ is

$$\alpha = \sum_{i=1}^{n} a_i b_i,\tag{1}$$

where the coefficients  $a_i(x)$  are univariate polynomials over  $F_q$  and the standard representation is typically exponential in the size of the field, so powering units requires a very large amount of space and time. In order to practically solve norm equations over function fields, it is favourable to have a shorter representation for units.

In general, a compact representation of  $\alpha \in O_F$  is defined as a vector of elements of F [2]:

$$\mathbf{t}_{\alpha} = (\gamma, \beta_1, \beta_2, \cdots, \beta_l) \tag{2}$$

that satisfies a power product with integer exponents  $\lambda_i$ , typically  $2^{l-i}$  for  $i \in \{1, 2, \dots l\}$ ,

$$\alpha = \gamma \prod_{i=1}^{l} (\beta_i)^{\lambda_i} \tag{3}$$

where  $\gamma$  and  $\beta_i$  are elements of *F* that satisfy certain conditions. The form of equation 3 enables to compute multiplication and exponentiation in less time which consume a lot of time when using standard representation.

This work represents a part of my doctoral dissertation under the supervision of Dr. Renate Scheidler and Dr. Michael Jacobson.

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## A Computational Comparison of Inverse Problem Techniques, Young and Old

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A goal of many inverse problem techniques is to find unknown parameter values  $\lambda \in \Lambda$  that produce a solution to the forward problem,  $u_{\lambda}$ , that lies "close" to a known solution, u. Mathematically speaking, these techniques wish to minimize the approximation error,  $||u - u_{\lambda}||$ .

A number of different inverse problem techniques have been developed for solving such a problem, perhaps the most popular of which is Tikhonov regularization. Regularization techniques often cast the above problem in terms of a linear system Af = d, where A is an operator containing known information, d contains known information, and f contains the unknown parameters. As the operator A is often not invertible, or does not have a bounded inverse, the problem of solving for f is ill-posed. Regularization schemes replace the ill-posed operator with a "nearby" well-posed operator and then add a penalty (or regularization) term to correct for this adjustment.

Iterative Schemes are also prevalent in the inverse problem literature. As their name implies, an iteration scheme is developed that is designed to converge to a solution (after a large number of iterations) that is "close" to the true parameter values. One such iteration scheme is explored in this talk, Landweber-Fridman iteration.

A more recent inverse problem technique is that of Collage-coding. The idea behind this technique is to bound the approximation error above by another distance that is more easily minimized. When working with ODEs, this upper bound is achieved using the Collage Theorem, a consequence of the well-known Banach's Fixed Point Theroem,

$$\|u-u_{\lambda}\|\leq \frac{1}{1-c_{\lambda}}\|u-T_{\lambda}u\|,$$

where  $T_{\lambda}$  is a  $c_{\lambda}$ -contractive, space preserving operator that depends on the unknown parameters  $\lambda$ . By minimizing the so-called collage distance  $||u - T_{\lambda}u||$  (ensuring that  $c_{\lambda}$  is bounded away from 1), one can ensure that the approximation error is indeed small. Relying instead on the Lax-Milgram Representation Theorem, Collage-coding methods have been developed for both linear and nonlinear PDEs.

In this talk, we will compare and contrast each of these methods by applying them to the same set of examples. The accuracy, robustness, and efficiency of each method will be explored.

#### Mean-square stability of stochastic system with impulse and unbounded delay

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This paper investigates mean-square stability of stochastic system with time-varying parameters, impulses and unbounded delay. Applying the characteristics of two kinds of impulses, stochastic analysis techniques and mathematical deduction, the two conclusions on mean-square stability analysis of the considered system are obtained. Then the controller is designed for time-invariant system with unbounded time delay and impulses.

The following stochastic time-varying systems with impulses and time-varying unbounded delay is considered,

$$\begin{cases} dx(t) = (A(t)x(t) + B(t)x(t - \tau(t)))dt + (C(t)x(t) + D(t)x(t - \tau(t)))dw(t), & t > t_0 \\ x(t_k) = \alpha_k x(t_k^-), & k \in N^+ \\ x(t) = \phi(t), & t \in [t^0, t_0], \end{cases}$$
(1)

where  $x = (x_1, ..., x_n)^T \in \mathbb{R}^n$ ;  $A(t) = [a_{ij}(t)], B(t) = [B_{ij}(t)], C(t) = [c_{ij}(t)], D(t) = [d_{ij}(t)] \in C([t_0, +\infty), \mathbb{R}^{n \times n})$ ;  $\tau(t) \ge 0$  is a continuous time delay,  $\alpha_k \in \mathbb{R}^+$  for any  $k \in N^+$ ,  $\phi = (\phi_1, ..., \phi_n)^T \in C([t^0, t_0], \mathbb{R}^n)$ ; w(t) is a onedimensional  $\mathscr{F}_t$ -adpated Brown motion defined on the complete probability space  $(\Omega, \mathscr{F}, \{\mathscr{F}_t\}_{t \ge t_0}, P)$ ; and  $t^0 = \inf_{t \ge t_0} \{t - \tau(t)\}$ .

Based on the system (1), the several main results are given,

Lemma 1: If these is a function  $\psi(t) \in \Psi$  such that  $b(t) \frac{\psi(t)}{\psi(t-\tau(t))} + a(t) < 0, t \ge t_0$ , then we have  $E|x(t)|^2 \le \tilde{X}(t_0)\chi_k\psi^{-1}(t)$ . for  $t \in [t_0, t_k)$ . Where  $a(t) = \max_{i \in \mathcal{N}} \{\upsilon_{ii}(t) + \sum_{j=1, j \ne i}^n |\upsilon_{ij}(t)| + \sum_{j=1}^n |\theta_{ij}(t)|\} < 0, b(t) = \max_{i \in \mathcal{N}} \{\sum_{j=1}^n |\theta_{ji}(t)| + \sum_{j=1}^n |\pi_{ij}(t)|\}, \mathcal{N} = \{1, ..., n\}, \tilde{X}(t_0) = \sup_{h \in [t^0, t_0]} E(x^T(h)x(h)), \chi_0 = 1, \chi_k = \prod_{i=0}^{k-1} (1 \lor \alpha_i^2), k \ge 1.$ 

Theorem 1: If the impulses are all stabilizing or there are only finite destabilizing impulses, then under conditions in Lemma 1, the systems (1) can achieve mean-square exponential stability or polynomial stability if  $\psi(t) = e^{t-t_0}$  or  $\psi(t) = t - t_0 + 1$ .

Lemma 2: If there are constants  $\lambda > 0, \beta > 1$  and  $\overline{\omega} \in (0, \lambda)$  such that  $b(t)\beta^{\lambda\tau(t)} + \lambda \ln\beta + a(t) < 0$  and  $|\alpha_k| \le \beta^{\frac{1}{2}\overline{\omega}(t_{k+1}-t_k)}$ . Then we have

$$\beta^{\lambda(t-t_0)} E(x^T(t)x(t)) \le \tilde{X}(t_0) \beta^{\varpi(t_k-t_0)}, \ t \in [t_{k-1}, t_k), k \in N^+.$$
(2)

Theorem 2: Let the maximum impulse time interval  $T_{\max} = \sup_{k \in N^+} \{t_k - t_{k-1}\} > 0$ , under the same conditions as Lemma 2, the conclusion (2) is equivalent to  $E|x(t)|^2 \leq \bar{\beta}\tilde{X}(t_0)\beta^{-(\lambda-\bar{\omega})(t-t_0)}$ , for any  $t \geq t_0$ , where  $\bar{\beta} = \beta^{T_{\max}} > 1$ , which means that the trivial solution is mean-square stable.

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### **Compensated Compactness, Isometric Immersions, and Physical Applications**

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We present some recent results ([1, 3, 6]) on geometric compensated compactness theorems and their applications in differential geometry, nonlinear elasticity and physical PDEs.

The theory of compensated compactness has played a central rôle in the study of gas dynamics, hyperbolic conservation laws and continuum mechanics (*cf.* Dafermos [5] and Tartar [7]). For the purpose of applications in problems of differential geometry, we developed geometric versions of generalised compensated compactness theorems, *e.g.* for differential forms on Riemannian manifolds, and for sections of vector bundles over semi-Riemannian manifolds. They serve as the key tool for establishing the weak stability of  $W^{2,p}$ -isometric immersions — or, the weak stability of the  $L^p$ -solutions for Gauss–Codazzi–Ricci equations — of (semi)-Riemannian manifolds into (semi)-Euclidean spaces; see [1, 3] and expositions in [2].

On the other hand, the aforementioned geometrical perspectives in turn enable us to further explore the compensated compactness theory from the harmonic analytic point of view, a la Coifman–Lions–Meyer–Semmes [4]. In [3], a compensated compactness theorem on *LCA* (locally compact abelian) groups was obtained; also, in [6] we developed the div-curl lemma for differential forms on manifolds of bounded geometry, and proved the div-curl atomic decomposition of the local Hardy space (defined via maximal characterisation) over such manifolds.

Finally, despite the abstract nature of the above results, various applications have been found in problems of physics and engineering. In particular, we addressed the weak stability properties of Einstein's structural equations and the asymptotic rigidity phenomena in nonlinear elasticity using our generalised compensated compactness theorems.

Related open problems will also be briefly discussed.

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## Data Visualization Techniques for Single and Multiple Spike Trains

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With the rapidly growing data collection technologies in simultaneous recording of large populations of neurons, it is crucial to develop statistical techniques for data analysis. Data visualization is a powerful exploratory tool to gain insight into multi-dimensional spike trains, and to detect informative spiking patterns/relationships. This talk summarizes some of the literature on visualization techniques for neural spike trains. We focus on detecting informative patterns, e.g. periodicity and burst spiking, in single neurons as well as on identifying synchronous firings in neuronal populations. We also address the computational challenges in information visualization for simultaneously recorded neural spike trains, and offer solutions in a couple of studies involving decision-making and visual stimulation. Through a simulation study, the pros and cons of different techniques are demonstrated and compared.

## Highly Accurate Numerical Simulation of Acoustic Wave Equation with Perfectly Matched Layer Boundary Condition

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In this work, we present a highly accurate finite difference method to solve the 2D acoustic wave equation

$$\rho(\mathbf{x})\partial_t^2 u(\mathbf{x},t) + \nabla \cdot (\kappa(\mathbf{x})\nabla u(\mathbf{x},t)) = f(\mathbf{x},t), \ (\mathbf{x},t) \in \Omega \times (0, T_f],$$
(1)

where  $\rho$  and  $\kappa$  are the density and bulk modulus of the medium, respectively. **x** is the spatial variable in 2D domain  $\Omega$ . The Perfectly Matched Layer (PML) boundary condition is specified to absorb boundary reflections. Due to the heterogeneity of the medium, both density and acoustic velocity are location dependent functions, therefore, the widely used high-order compact schemes cannot be used directly for higher-order accuracy.

To overcome this problem, we first extend the numerical scheme developed in [3] to the wave equation (1) with PML boundary condition. To obtain higher order accuracy and efficiency, we still adopted the so-called combined compact scheme[2, 1], which was originally introduced to approximate first and second derivatives with high-order accuracy using a compact stencil. The time integration is also implemented using higher-order Runge-Kutta method. Several numerical examples have been conducted to demonstrate the overall efficiency and high accuracy of the new method.

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## **Population Motivated Discrete-time Disease Models**

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We introduce the Susceptible-Infected-Removed (SIR) model, the Susceptible-Exposed-Infected-Removed (SEIR) model coupled with a social mobility model (SMM). We discretize them by a Forward Euler Method, which can be viewed through a mean-field approximation from a discrete version. We calculate basic reproduction number  $R_0$  using the next generation matrix method. Then we obtain hyperbolic forward Kolmogorov equations (high-dimensional PDEs) and show that its projected characteristics corresponding to these models coincide with population motivation. Finally, we use the Deep Galerkin Method (DGM) to solve the high order nonlinear PDEs. In this project, we can improve the global prediction of epidemics dynamics, which can provide suggestions on "how to control " epidemics. In addition, we also use these methods to solve the Cancer Immunotherapy model, which can provide another way to observe the blockade of immune checkpoints in the tumor dynamics.

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#### **Radiation Modeling in Laser Fusion Simulation**

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Radiation modeling is very important in the simulation of laser inertial confinement fusion (ICF) [1], in which a high power laser is used as a driver to implode capsules filled with fusion fuel and to produce thermonuclear energy. Radiation transport plays an important role in energy transport for a capsule implosion. Good understanding of radiation transport can help us a lot in design of laser ICF ignition target.

The numerical difficulties in solving the transport equation stem from the fact that the absorption and emission coefficients not only determine the radiation field, but are usually to a significant extent determined by the radiation field [2]. Generally, there are four kinds of physical model for radiation: thermal conduction model, three-temperature model, multi-group diffusion model, and multi-group transport model. Diffusion and transport methods are commonly used in laser ICF simulation. The diffusion method is by far the most important approximation treatment of radiation transport, and is found to be so much simpler than solving the full transport equation. It is well known that a diffusion model is a good approximation for high-Z and high density materials, while a transport model should be used for simulation of low-Z and low density materials. Generally, transport model is better than diffusion model. However, transport model is much CPU time consumed than diffusion one.

We propose a hybrid transport-diffusion method to keep better modeling without much CPU time consumed. For a computation domain composed of diffusion and transfer regions, we use a domain decomposition method for solving radiation hydrodynamics equations. Diffusion and transfer regions are solved separately. Multi-group flux-limited diffusion method is used in diffusion regions, while multi-group Discrete Ordinate  $S_N$  method in transfer regions. A key point in our method is to build a connection condition between a diffusion region and a transfer region, i. e., the boundary condition for a region should be given according to its two neighbours. The boundary condition for a diffusion region is easily given from a transfer region by using radiation flux continuity condition. However, as the boundary condition for a transfer region, radiation intensity should be constructed according to radiation energy density of its neighbour diffusion regions. We will present our hybrid transport-diffusion method, and show some simulation results on interaction of radiation with low-Z foam, mid-Z matter, and high-Z matter by using multi-group diffusion, multi-group transport, and hybrid transport-diffusion radiation methods.

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## "Range-based function approximation" using measures in range space and generalized Weber's model of perception

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We have been interested in the problem of function approximation using metrics which permit differing degrees of deviation according to the function values. A primary motivation is Weber's (generalized) model of perception: Given a greyscale background intensity I > 0, the minimum change in intensity  $\Delta I$  perceived by the human visual system (HVS) is related to I by  $\frac{\Delta I}{I^a} = C$ , where a > 0 and C is a constant, or at least roughly constant over a significant range of intensities I. The case a = 1 corresponds to the standard Weber model which is employed in most, if not all, applications. A Weber-conforming, or "Weberized," distance between two functions u and vshould tolerate greater (lesser) differences over regions in which they assume higher (lower) intensity values.

In this talk, we describe a general mathematical method of constructing "Weberized" metrics over function spaces by means of measures over the range space,  $\mathbb{R}_g$ , of the functions. Very briefly, let  $\mathscr{F} = \{u : X \to \mathbb{R}_g \mid u \text{ is measurable }\}$  be the signal/image function space, where X = [0, 1] and  $\mathbb{R}_g = [A, B] \subset (0, \infty), A > 0$ . Given two functions  $u, v \in \mathscr{F}$ , define the following subsets of  $X: X_u = \{x \in X \mid u(x) \le v(x)\}$  and  $X_v = \{x \in X \mid u(x) \le v(x)\}$ . Now let v be a measure over (Borel subsets of) the range space  $\mathbb{R}_g$  and define the following distance between uand v associated with the measure v,

$$D(u,v;v) = \int_{X_u} v(u(x),v(x)] dx + \int_{X_v} v(v(x),u(x)] dx.$$
 (1)

In the case that  $v = m_g$ , (uniform) Lebesgue measure on  $\mathbb{R}_g$ , then  $D(u, v; m_g) = d_1(u, v)$ , the standard  $L^1$  distance between *u* and *v*. In the more general case that *v* is defined by a continuous density function  $\rho(y)$ ,  $y \in \mathbb{R}_g$ , then

$$D(u,v;v) = \int_{X} |P(u(x)) - P(v(x))| dx, \text{ where } P'(y) = \rho(y).$$
(2)

In the special case,  $\rho(y) = 1/y$ , we show that the resulting  $L^1$ -logarithmic distance function may be viewed as conforming to Weber's model, where a = 1, in terms of an exact "equal-area condition" involving  $\rho(y)$ . (Note that, as expected, the weighting decreases with increasing greyscale value.) We then apply this equal-area condition to the general case  $a \in (0, 1)$  and show that to leading order,  $\rho_a(y) \sim 1/y^a$  as  $y \to \infty$ . (It is also possible to determine all subdominant corrections.)

Finally, let u(x) be a reference function and  $v(x) = \sum_{k=1}^{N} c_k \phi_k(x)$  an approximation to u(x), where the set  $\{\phi_k\}_{k=1}^{N}$  is assumed to be linearly independent over X = [0, 1]. We denote  $Y_N = \text{span}\{\phi_1, \dots, \phi_N\}$ . It is more convenient to work with the  $L^2$ -analogues of the  $L^1$ -based distance functions in Eq. (2), i.e.,

$$D_{2,a}(u,v;v_a) = \left[\int_X [u(x)^{-a+1} - v(x)^{-a+1}]^2 dx\right]^{1/2}, \ a \in (0,1) \text{ and } D_{2,1}(u,v;v_1) = \left[\int_X [\ln u(x) - \ln v(x)]^2 dx\right]^{1/2},$$

where  $v_a$  is the measure on  $\mathbb{R}_g$  with density function  $\rho_a(y) = 1/y^a$ . We consider the best  $Y_N$ -approximation of u in the metric space  $(\mathscr{F}, D_{2,a})$  to be the function v which minimizes the "Weberized" distance  $D_{2,a}$ . (Note that in the case a = 0, i.e., an absence of Weber's model,  $\rho_0(y) = 1$  and  $D_{2,0}(u,v;v_0) = d_2(u,v)$ , the standard  $L^2$  distance.) Some numerical examples are presented to illustrate the method and the effect of "Weberizing" the metric.

#### **Quaternion Windowed Linear Canonical Transform of Two-Dimensional Signals**

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We investigate the 2D quaternion windowed linear canonical transform(QWLCT) in this paper. Firstly, we propose the new definition of the QWLCT, and then several important properties of newly defined QWLCT, such as bounded, shift, modulation, orthogonality relation, are derived based on the spectral representation of the quaternionic linear canonical transform(QLCT). Finally, by the Heisenberg uncertainty principle for the QLCT and the orthogonality relation property for the QWLCT, the Heisenberg uncertainty principle for the QWLCT is established.

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# Spatial Fourth-order and Temporal Second-order Conservative Characteristic Method for Environmental Modelling

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Modelling atmospheric environment is a difficult problem. The temporal and spatial variation of aerosols are influenced by numerous physical and chemical processes, such as emission, spatial advection and diffusion, aerosol dynamics and aerosol chemistry, etc. Aerosol transport computation may be carried out at continental or global scales for long term simulation, which would result in large scale computation. In this talk, we will present our new development of a spatial fourth-order and temporal second-order conservative characteristic finite volume method for solving atmospheric pollution convection diffusion problems. While the characteristics tracking is applied to treat the convection term, we use high-order conservative interpolation to treat the advective integrals over the irregular tracking volume cells at the previous time level. A temporal discretization by averaging along the characteristics is proposed for the diffusion term, where the diffusion fluxes are approximated by fourth-order spatial discrete operators that provide continuity of the discrete fluxes cross the edges of volume cells and tracking volume cells. Numerical experiments verify the temporal and spatial accuracies as well as mass conservative property. Realistic atmospheric pollution problems are further simulated by the developed conservative algorithm.

## High-Order Numerical Methods for Good Boussinesq Equations

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The solitary wave interaction mechanism for the good Boussinesq equation is complicated. Solitary waves only exist in a finite range of wave speeds. Large solitons can turn into anti-solitons, while small solitons remain stable. It is also possible for solitons to merge and split.

In this talk, high order numerical schemes for the good Boussinesq equations are studied. We shall construct a 3rd-order time splitting spectral method via splitting the good Boussinesq equation into a system which consists of a linear equation and a nonlinear ODE. This resulted linear equation can be solved via spectral method while the nonlinear ODE can be solved exactly. The total error comes mainly from the splitting error which is 3rd order based on our construction. Numerical simulations to check convergence order and for solitary wave interaction shall be performed.

## Stability criteria of hybrid dynamical systems in terms of two measures $_{\rm X.\ Liu^1}$

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

## Deterministic and Stochastic Models of Spontaneous Cell Polarization

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Cell polarity intrinsically lies at the localization of signaling molecules on certain regions of membrane. The localization is formulated by the diffusion or reaction of signaling molecules. Without the guiding cue, cell can also go through the process spontaneously. This spatio-temporal dynamics of polarizing system has been largely investigated by reaction-diffusion equations (RDEs), especially Turing mechanism (see Ref. [1]) and wave-pinning mechanism (see Ref. [2]) for the emergence of pattern formation. Besides these deterministic models, the onset of polarity has been described stochastically through compartment-based or particle-based methods.

Our study by performing Gillespie stochastic simulation algorithm (SSA), reveals the stochastic model leads to wider parameter ranges for cell polarization with different feedback forms compared to deterministic system. This underlies noise promotes the emergence of pattern formation, in contrast to the phenomenon that fluctuation in wave-pinning system acts as a destabilizing agent. Although the effect of intrinsic fluctuations can be visualized by numerical simulations (see Fig. 1), to quantitatively measure its effect, we progress by doing van Kampen system size expansion (see Ref. [3]) and adopting the power spectrum of signaling molecule species. This gives us insight on how fluctuation behaves during the cell polarizing process especially at low number of molecules. At some parameter sets where SSA succeeds but RDEs fail in the emergence of cell polarization, the power spectrum shows a peak profile which indicates the presence of intrinsic noise. Our analytical investigations of power spectrum verify the noisy performance we have observed in stochastic simulations. These results provide an insight on the role of noise in biology morphology.

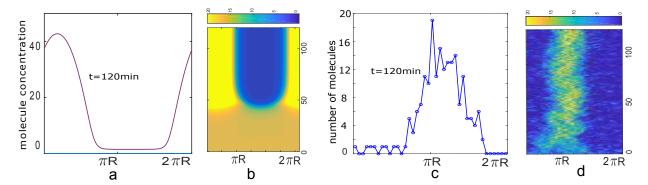


Figure 1: The dynamics of active molecule in deterministic (in **a** and **b**) and stochastic (in **c** and **d**) models within 120 minutes.

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## Poiseuille flow of nematic liquid crystals via Ericksen-Leslie model

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Abstract: In this talk, we will discuss a recent global existence result on the Poiseulle flow of nematic liquid crystals via full Ericksen-Leslie model. The existing results on the Ericksen-Leslie model for the liquid crystals mainly focused on the parabolic and elliptic type models by omitting the kinetic energy term. In this recent progress, we established a new method to study the full model. A singularity formation result will also be discussed, together with the global existence result showing that the solution will in general live in the Holder continuous space.

### Topological models of superconducting quantum circuits

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Exploiting the tunability of the qubit frequency and qubit-qubit coupling, we show that a superconducting qubit chain can simulate various topological band models. When the system is restricted to the single-spin excitation subspace, the SSH model (Su-Schrieffer-Heeger model) can be equivalently simulated by alternating the coupling strength between neighboring qubits. The topological edge states and pumping are studied. We also study the quantum coherence in a qubit chain and find that the quantum coherence might be topologically protected.

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# Stability and stabilization of chaotic systems under aperiodic sampling and state quantized controller

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This study aims at investigating the problem of stability and stabilization of chaotic systems on the basis of T–S fuzzy model under aperiodic sampling and state quantized controller. A modified Lyapunov-Krasovskii functional (LKF), which fully captures the information of the sampling pattern, is constructed to the chaotic systems. Together with free-weighted matrices technique, much less conservative stabilization results are derived in term of linear matrix inequalities (LMIs). A numerical example is presented to show the effectiveness of the proposed method.

#### System Model

Consider the following nonlinear chaotic system:

$$\dot{x}(t) = f(x(t), u(t)),$$
 (1)

where  $f(\cdot)$  denotes the known nonlinear function,  $x(t) \in \mathbb{R}^n$  is the state vector,  $u(t) \in \mathbb{R}^m$  denotes the control input. The nonlinear system (1) can be described as the following T–S fuzzy model:

**Plant rule** j : IF  $\beta_1(t)$  is  $\gamma_{i1}$ ,  $\beta_2(t)$  is  $\gamma_{i2}$ ,... and  $\beta_r(t)$  is  $\gamma_{ir}$ , THEN

$$\dot{x}(t) = A_j x(t) + B_j u(t), \quad j = 1, 2, \dots, s,$$
(2)

where  $\beta_1(t), \beta_2(t), \ldots, \beta_r(t)$  denote premise variables,  $x(t) \in \mathbb{R}^n$  denotes state vector,  $u(t) \in \mathbb{R}^m$  is control input.  $\gamma_{ji}$  are fuzzy sets,  $j = 1, 2, \ldots, s, i = 1, 2, \ldots, r, A_j$  and  $B_j$  are known matrices with appropriate dimensions, *s* is the number of IF-THEN rules.

Let  $\beta(t) = [\beta_1(t), \beta_2(t), \dots, \beta_r(t)], \alpha_j(\beta(t)) = \frac{\prod_{i=1}^r \gamma_{ji}(\beta_i(t))}{\sum_{j=1}^s \prod_{i=1}^r \gamma_{ji}(\beta_i(t))}$  with  $\gamma_{ji}(\beta_i(t))$  is the grade of membership of  $\beta_i(t)$ 

in  $\gamma_{ji}$  and presume that  $\prod_{i=1}^{r} \gamma_{ji}(\beta_i(t)) \ge 0$ ,  $\sum_{j=1}^{s} \prod_{i=1}^{r} \gamma_{ji}(\beta_i(t)) > 0$ ,  $\forall t > 0$ ,

$$\alpha_j(\boldsymbol{\beta}(t)) \ge 0, \quad \sum_{j=1}^s \alpha_j(\boldsymbol{\beta}(t)) = 1.$$
(3)

By fuzzy blending, the fuzzy system (4) can be inferred

$$\dot{x}(t) = \sum_{j=1}^{s} \alpha_j(\beta(t)) [A_j x(t) + B_j u(t)].$$
(4)

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### **Predicting Cardiac Arrest Using Convolution Neural Networks**

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**Background:** Dialysis is life saving treatment for renal failure patients, but has serious side effects which may lead to cardiac arrest. ECG is the most widespread non-invasive clinical measurement, we aim to ascertain the relationships between dialysis parameters and cardiac arrest. To do so, we applied ECG-based convolutional neural network to cardiac arrest prediction.

**Methods:** To construct inputs for the network, a large amount of ECG data was obtained from an open source ECG repository, i.e. the MIT-BIH Arrhythmia Database [1, 2]. The data is composed of 48 half-hour excerpts of two-channel ambulatory ECG recordings with beat and rhythm labels. The ECG data was first detrended, denoised and segmented to extract cardiac features including but not limited to the QRS duration, T waves and QT intervals. With the ECG data and the cardiac features, we developed and trained the convolutional neural network [4] to output the cardiac arrest probability alongside the probability of other cardiac arrest indicators, such as ventricular fibrillation. The main machine learning system we used was TensorFlow [3] which focuses on training and inference on deep neural networks. With guarantee of the model's high accuracy and avoidance of overfitting, we inputted the ECG data from the same patient group before and after dialysis to the CNN in comparison of their cardiac arrest probability. For improvement of the Deep Learning model and increase in the accuracy, a deep convolutional neural network with residual connections [5] was developed to estimate the cardiac arrest probability in parallel, and a LSTM neural network is also under construction to utilize the time-dependent nature of ECG.

**Results:** In our preliminary simulations, the before-after cardiac arrest probability alongside the probability of other cardiac arrest indicators in the same patient group had an apparent increase in two different convolutional neural network models.

**Conclusions and Discussion:** Though different neural networks possessed different prediction accuracy, dialysis always increases the likelihood of cardiac arrest, which strongly indicates the detriment of dialysis.

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#### An Implementation of LCAO Time-Dependent DFT in the Optical Limit

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We present here work done towards the development of a time-dependent density functional theory (TDDFT) code implemented in the GPAW environment [1]. The linear combination of atomic orbitals (LCAO) decomposition for our wavefunctions is used [2], and our optoelectronic response functions are calculated in reciprocal k and frequency  $\omega$  space in the optical limit of zero wavenumber. The motivation for writing this code rests in a growing interest in the nanophotonics and biological communities in purely optical response functions for large macromolecular systems, whereas, due to computational issues, other TDDFT implementations in GPAW become intractable for such large systems. Utilizing LCAO provides an impressive computational speedup with a minor trade-off in terms of accuracy. We have also developed methods that provide a spatially-resolved view of the relevant electron transitions for any given material. These methods can be used in tandem with experimental results to provide an atomically-resolved description of electron energy loss spectroscopy results [3].

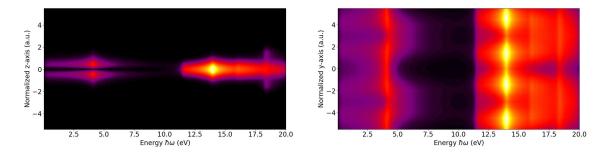


Figure 1: Projection of the electron density onto the axis normal to graphene (left) and the axis passing through two neighboring C atoms (right) as a function of energy  $\hbar\omega$  for single layer graphene. The shape of the  $p_z$ -orbital can be clearly seen near 4 eV and the broader excitation near 14 eV suggests electrons active in the hybrid in-plane  $\sigma$  orbitals contribute most to excitations in this region. The distance along the axes is given in atomic units (a.u.).

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# Model Predictive Control Implementation for a Quadruple-Tank System Using Arduino

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Programmable logic controllers (PLC) are widely used in industry; however, in the academy, its use is limited mainly because of economic or license restrictions. The present work aims to show an alternative to the use of commercial PLC employing open-source hardware and software such as Arduino and Python, making it affordable for a large number of students. Quadrupletank system, Fig. 1, was selected due to its non-linearity and capability to operate in both minimum and non-minimum phases [1]. Four equations describe this system [2].

Model Predictive Control (MPC) is a modern control method that uses a mathematical model to predict outputs depending on the known values up to instant t and on the future control signals, these control signals are calculated by optimizing an objective function [3].

Based on this model, we control the level of the tanks by using MPC programmed on a PC, which is our PLC: input signals from the ultrasonic level sensor connected to the Arduino Uno board are received and shared with Python to calculate the objective function and control law to send these control signals to the electromechanical valve.

Once the adjustment of the control parameters has been done, it is observed that the set-point values are quickly reached, this behavior is observed in Fig. 2.

Finally, it is concluded that low-cost implementation of this type of control for academic purposes is feasible allowing students to analyze these non-linear systems.

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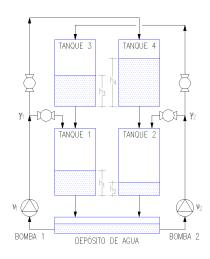


Figure 1: Quadruple-tank system.

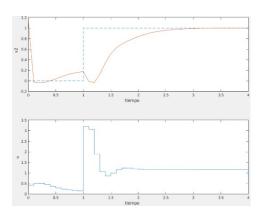


Figure 2: Above: Process values are shown in continue red line and set-point value in dotted blue line. Below: Step response of control output variable

### Strategy-proofness and perfect mechanisms

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We introduce the notion of a *perfect mechanism*—a structured pair consisting of (i) a dynamic perfect information game form, and (ii) a *convention* specifying an *honest strategy* for each player given his type—to establish the existence of socially optimal ex-post perfect equilibria in a large class of dynamic games where the agents may have extremely limited information about the economy. Applications include marriage markets with dating apps, labor markets with telephones, and online auctions.

# **Divisor Class Group Arithmetic on** C<sub>3,4</sub> **Curves**

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Computing in the divisor class group of an algebraic curve is a non-trivial component in computing the curve's *L*-series. *L*-series, in turn, are at the heart of many number theoretic conjectures, including the Sato-Tate conjecture and its generalization to other families of curves [6]. In order to test these conjectures against other curve families, it is desirable to have efficient algorithms to perform arithmetic in the divisor class group of those curves.

Fast explicit formulas exist to perform divisor class group arithmetic for genus 1 and genus 2 curves. However, the picture for genus 3 curves is incomplete. Existing explicit formulas for arithmetic on non-hyperelliptic genus 3 curves ( $C_{3,4}$  curves) have been developed with cryptographic applications in mind [1, 2, 3, 5]. They make certain generacity assumptions on their inputs that hold with high probability for curves over a sufficiently large finite field, but they are not suitable for number theoretic use cases where one might operate over smaller base fields. Where the cryptographic algorithms fail, slower, more general algorithms exist to perform divisor class arithmetic over any curve [4]. The goal of this project is to bridge the gap – to find fast explicit formulas describing  $C_{3,4}$  curve arithmetic that are correct for all inputs.

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# Numerical Method in Riemann Invariant Form for Investigating The Effectiveness of A Submerged Bar Breakwater Model as A Coastal Protector

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Recently, Geotextiles is widely used for coastal protection in Indonesia. The Geotextiles is one of the implementations of a submerged bar as a breakwater. Here, we will study the damping mechanism of a Geotextiles to the reduction of incoming wave amplitudes. The mathematical model that we use based on the shallow water type equation. We derived the analytical solution to obtain the transmission wave coefficient. Numerically, we construct a numerical method in the form of Riemann invariant. We will present the advantage of working with the Riemann formulation. For validation, we compare our numerical result with the analytical wave transmission coefficient. Moreover, we investigate the optimal dimension of a submerged bar for an incoming wave with a specific wavelength to get the minimum amplitude of the transmitted wave.

# Statistical and Computer Models for Geophysical Mass Flows

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Rare natural hazards such as large volcanic eruptions can cause loss of life and damage to property. With sufficient information, those charged with public safety may issue warnings of impending hazards to mitigate the hazard impact. Recent developments in modeling and simulating large geophysical mass flows can provide useful information in assessing hazard risk. In particular, computer simulations of a model system of PDEs, which determines flow depth and runout, are expensive to run. On the other hand, analysis based on only a few simulations is not sufficiently accurate for hazard analysis. Computational costs can be reduced by constructing a statistical emulator -an approximate response surface for selected output variables derived from several full simulator runs. Whenever the result from a simulation is required in an analysis, the emulator can be queried quickly. A key feature of the emulator is that an estimate of the prediction uncertainty is defined together with the regression estimate. A popular emulator is the Gaussian Separable Process emulator, or GaSP, which is constructed as the mean of a Bayesian posterior distribution over outputs. In this work, we propose an alternative procedure for constructing emulators, one that uses knowledge about the model physics. We model the mass flow as an Ornstein–Uhlenbeck (OU) process for sliding blocks over the topography. We demonstrate how the OU results can be used to predict simulator results. By calibrating certain input parameters, a fit to the OU process is made, together with an error approximation, by classical statistical techniques, to provide an emulator of the runout computed by the computer simulator.

#### Landscape similarity analysis: comparing hand-crafted and learned features

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Landscape similarity mapping is becoming increasingly important and complex as high-resolution remotely sensed datasets become more widespread. With the availability of such data, there are new opportunities to monitor how environment and ecosystems are influenced by natural and anthropogenic processes. For example, we might be interested in querying all image scenes to assess their similarity to a scene that was disturbed by a wildlife. Alternately, landscape remediation may seek to quantify how similar a site is to a natural site after resource extraction. While the applications for landscape similarity analysis are vast, sensor viewing angle, illumination, shadows, noise and other environmental factors however render landscape similarity analysis cumbersome. A common approach is to normalize the spectral space to generate radiometrically similar sequences of images. Object, contextual and textural information are recognized to hold potential for addressing the aforementioned problems. Local binary patterns (LBP) are effective hand-crafted features used to represent local image texture and are successfully employed in change detection, classification and pattern recognition, and shown to outperform many other methods. Convolutional neural networks (CNN) have also revolutionized pattern detection tasks with their capability to extract rich features, which have intrinsic adaptation to alleviate illumination and translation invariance limitations of most classical methods. A CNN processes hierarchical feature maps given a sequence of input images. The lower layers extract spatially local information while later layers encode and retain more abstract global information. These maps can be useful templates for recognizing specific scenes or landscape patterns. While automating LBP applications can be challenging, high performing CNNs may be difficult to train as long training times and large annotated training samples are required. In this study, we compared LBP and a pre-trained CNN lower layer activations (feature maps) in a tundra ecosystem mapping application characterizing spatial distribution of ground lichen, shrubs and other landcover types. High-resolution unmanned aerial vehicle (UAV) imagery over the Arctic in North Western Territories, Canada was employed to compare the discriminative potential of learned vs. hand-crafted textureencoding features in the context of landscape similarity analysis. For each method, a template patterns is compared to a suite of images with varying levels of pattern similarity. Rankings of methods are compared and similarities and differences were quantified. We conclude with notes on practical implementation issues for landscape similarity analysis.

Keywords: Landscape patterns, local binary patterns, illumination invariant features, convolutional neural networks

#### Long-time asymptotics for the focusing nonlinear Schrödinger equation and the nonlinear stage of modulational instability

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#### Abstract

The focusing nonlinear Schrödinger (NLS) equation on the whole line with initial data that do not vanish at infinity is analyzed asymptotically in the limit  $t \to \infty$  via the inverse scattering transform and the Deift-Zhou method for oscillatory Riemann-Hilbert problems. First, attention is given to the case of data such that no discrete spectrum arises in the inverse scattering transform. It is then shown that, depending on the value of the similarity ratio x/t, the leading-order solution is described by either a plane wave or a modulated elliptic wave whose amplitude involves the standard snoidal elliptic solutions of the focusing NLS equation. Next, the assumption of empty discrete spectrum is dropped, therefore allowing one to rigorously study the interaction between solitons and radiation in modulationally unstable media.

# Information Geometric and Probability Models for Multiple Neurons

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The activity of sets of neurons can be modelled, in a probabilistic way, by characterising the joint distribution of high-dimensional binary random variables. The set of possible models is very large and considerable insight can be gained by analysing the underlying geometry of this set. Possible geometric structures have been studied in the classical Information Geometry (IG) framework. After a brief review of this approach, we explore recent developments in IG which have moved away from differential geometry to include ideas from affine and convex geometry. We briefly discuss the advantages of this new approach to IG and its implications in neuroscience applications.

# **Integrated Information Theory – A Mathematical Model of Consciousness**

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In recent years, the science of consciousness has made substantial progress studying behavioural and neural correlates of consciousness; however, such approaches are limited to relatively healthy adult humans. These methods have little to say in many other situations of interest, such as vegetative state patients, infants, non-human animals, and artificial intelligence. To move beyond the correlative approach and address these difficult questions, there is need for a general theory of consciousness.

Integrated Information Theory (IIT) takes an axiomatic approach, proposing a set of properties that are true of every conscious experience [1]. These axioms are then translated into a set of postulates about the physical systems that support conscious experience, forming the basis for a mathematical model of consciousness. This talk will review the core mathematical ideas of IIT, including the notion of integrated information ( $\Phi$ ), which quantifies the extent to which a system is 'greater than the sum of its parts'.

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#### **Continued fractions in imaginary quadratic fields**

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In the Euclidean imaginary quadratic fields, continued fractions have been used to give rational approximations to complex numbers since the late  $19^{th}$  century [2]. A variety of algorithms (for example [1, 3, 4, 5, 6, 7, 8, 9]) have been proposed in the 130 years following their introduction, but none are applicable outside of the same five fields. We aim to overcome the non-Euclidean obstacle. We show how continued fractions can be produced in any imaginary quadratic field, and that they share many of the properties enjoyed by their classical forebear. The inspiration for the algorithm is a fractal arrangement of circles arising from subsets of  $GL_2(\mathbb{C})$  acting on the Riemann sphere [10]. The geometry of these arrangements reveals an analog of the Euclidean algorithm that points us toward a more general continued fraction.

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#### The Cutoff Paradox in the Kansas Presidential Caucuses

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The Kansas Republican Party uses an apportionment method of its own invention to apportion delegates to candidates in its presidential caucus. This method includes a threshold that eliminates candidates (and their votes) who receive less than 10% of the vote. Eliminating candidates can lead to a *Cutoff paradox*, a paradox in which a surviving candidate receives fewer delegates as a result of the elimination of the candidates that fall beneath the threshold. We provide a formula for the proportion of elections that are susceptible to this paradox for three candidate elections using the method of the Kansas Republican Party. For comparative purposes, we also provide a formula for the proportion that are susceptible to this paradox for themethod used by the Democratic Party in all of its presidential primaries and caucuses. Furthermore, we relate the Cutoff Paradox to the *No-Show Paradox*, a paradox in which lowering a single candidate's vote total results in an increase in that candidate's delegate allocation.

Our results demonstrate strong evidence that the method used by Kansas Republicans is far more susceptible to both the Cutoff Paradox and the No-Show Paradox than the method used by Kansas Democrats.

#### The least primitive root and Grosswald's conjecture

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Let *p* be an odd prime. A classical problem in analytic number theory is to give an upper bound on the least primitive root modulo *p*, denoted by g(p). In the 1960s Burgess proved that for any  $\varepsilon > 0$  one has  $g(p) \ll p^{1/4+\varepsilon}$  for sufficiently large *p*. This was a consequence of his landmark character sum inequality, and this result remains the state of the art. However, in applications, explicit estimates are often required, and one needs more than an implicit constant that depends on  $\varepsilon$ .

In 1952 Grosswald showed that if  $g(p) < \sqrt{p} - 2$ , then the principal congruence subgroup  $\Gamma(p)$  for can be generated by the matrix [1, p; 0, 1] and p(p-1)(p+1)/12 other *hyperbolic* matrices. Grosswald conjectured that  $g(p) < \sqrt{p} - 2$  for p > 409. Cohen, Oliveira e Silva, and Trudgian showed that this holds except possibly when  $p \in (2 \cdot 10^{15}, 4 \cdot 10^{71})$ . Treviño, Trudgian, and the speaker resolved Grosswald's conjecture assuming GRH. The final part of our proof involves a hybrid of theory and computation to deal with the cases where p-1 has 12, 13, or 14 prime factors. We will highlight this computational component in the talk.

Recently, Trudgian and the speaker have given an explicit upper bound on g(p) that improves (by a small power of log factor) on what one can obtain using any existing version of the Burgess inequality. In particular, we show that  $g(p) < 2r2^{r\omega(p-1)}p^{\frac{1}{4}+\frac{1}{4r}}$  for  $p > 10^{56}$ , where  $r \ge 2$  is an integer parameter. Our method allows us to show that Grosswald's conjecture holds unconditionally for  $p > 10^{56}$ , improving on previous results.

# Separation of variables for the Hamilton-Jacobi equation for the charged particle orbits for the Liénard-Wiechert potential in Minkowski space

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We use the theory developed by Benenti, Chanu and Rastelli [1] to study the problem of separation of variables for the Hamilton-Jacobi (HJ) equation for the charged particle orbits in the electromagnetic field generated by a moving charge in Minkowski space. A necessary condition for separation is that the field admits Killing vectors as symmetry operators. This condition imposes strong restrictions on the world line of the charged particle. We show that the HJ equation for the field generated by the Cavendish-Coulomb potential admits complete separation while that for a uniformly accelerated charge only admits partial separation.

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The V International AMMCS Interdisciplinary Conference Waterloo, Ontario, Canada Minisymposium (ID: SS-MMLSM) April 29, 2019

# An *in Silico* Analysis of Hypoxia-Activated Prodrugs in Combination with Anti-Angiogenic Therapy through Nanocell Delivery

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Tumour hypoxia is a well-studied phenomenon with implications in cancer progression, treatment resistance, and patient survival. While a clear adverse prognosticator, hypoxia is also a theoretically ideal target for guided drug delivery. This idea has lead to the development of hypoxia-activated prodrugs (HAPs): a class of chemother-apeutics which remain inactive in the body until metabolized within hypoxic regions. In theory, these drugs have the potential for increased tumour selectivity and have therefore been the focus of numerous preclinical studies. Unfortunately, HAPs have had mixed results in clinical trials, necessitating further study in order to harness their therapeutic potential. One possible avenue for the improvement of HAPs is through the selective application of antiangiogenic agents (AAs) to improve drug delivery. Such techniques have been used in combination with other conventional chemotherapeutics to great effect in many studies. A further benefit is achieved through nanocell administration of the combination. In the following, a mathematical model is outlined and used to compare the predicted efficacies of separate vs. nanocell administration for AAs and HAPs in tumours. The model is experimentally motivated, both in mathematical form and parameter values. Preliminary results of the model are highlighted throughout which qualitatively agree with existing experimental evidence. The model predicts an increase in the efficacy of HAPs when combined with AAs and that the optimal administration method is through nanocell delivery.

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# Conditional Value-at-Risk hedging and related questions

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Hedging of options is one of the basic and comprehensive problems of mathematical finance. The most visible developments in this area during the last two decades were done by using the notion of partial/imperfect hedging. We formulate this problem as a possibility to create a terminal capital which is close enough to given contingent claim in some probabilistic sense. Such understanding of the problem explains clearly why a reasonable statistical technique properly works here creating new types of hedging like quantile, efficient etc. Due to developments of risk measures this problem became a risk measures insight.

In the talk we investigate the partial hedging problem using the widely accepted risk measure CVaR - Conditional Value at Risk. Besides option pricing and risk management, CVaR was recommended by the Basel III as a key risk measure for regulation needs in modern financial industry. We develop the partial hedging problem by constracting optimal strategies that minimize CVaR under initial budget constraints. The CVaR – minimization is achieved by means of the Neuman-Pearson test. In the framework of a two factor market model we derive CVaR – hedging strategies for call and spread options. We also show how to provide a reasonable estimation of such risk measures, discuss possible applications of our findings and provide their numerical illustrations.

We look forward to welcoming you in Waterloo, Canada at the AMMCS-2017 Conference!

# A numerical algorithm for computing the limit inferior and its probabilistic analysis

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The numerical computation of many asymptotic quantities involves an estimation of either a limit superior (lim sup) or limit inferior (liminf). Two specific examples of this include wavelet methods for estimating the (local) smoothness of a signal (function) and the numerical estimation of various fractal dimensions (e.g., box counting dimension) of either sets or signals. In practice the most commonly used tool for these estimates is a least-square line generated from a log-log plot of the data, which clearly is subject to well-known problems (e.g., strong outliers).

In this talk we propose a novel numerical method for estimating either the liminf or limsup and give a probabilistic analysis of the performance of our algorithm. Our iterative method involves a repeated use of least squares along with a data pruning step. We show that our method works almost surely under two natural models for "generic" (randomly generated) data. In addition, we give some examples to show how the method can fail and which illuminate some features of the data set which will likely result in success.

# A New Method of Modelling Tuneable Lasers with Functional Composition

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A new nonlinear model is proposed for tuneable lasers. Using the generalized nonlinear Schrödinger equation as a starting point, expressions for the transformations undergone by the pulse are derived for each component in the cavity. These transformations are then composed to give the overall effect of one trip around the cavity. The linear version of this model is solved analytically, and the nonlinear version numerically. A consequence of this model being nonlinear is that it is able to exhibit wave breaking which prior models could not. We highlight the rich structure of the boundary of stability for a particular plane of the parameter space.

### Invariant Manifolds in the HamiltonianâHopf Bifurcation

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We study the evolution of the stable and unstable manifolds of an equilibrium point of a Hamiltonian system of two degrees of freedom which depends on a parameter v. The eigenvalues of the linearized system are pure imaginary for v < 0 and complex with nonzero real part for v > 0. (These are the same basic assumptions as found in the Hamiltonian-Hopf bifurcation theorem of the authors.) For v > 0 the equilibrium has a two-dimensional stable manifold and a two-dimensional unstable manifold, but for v < 0 there are no longer stable and unstable manifolds attached to the equilibrium. We study the evolution of these manifolds as the parameter is varied. If the sign of a certain term in the normal form is positive then for small positive v the stable and unstable manifolds of the system are either identical or must have transverse intersection. Thus, either the system is totally degenerate or the system admits a suspended Smale horseshoe as an invariant set. This happens at the Lagrange equilibrium point  $\mathcal{L}_4$  of the restricted three-body problem at the Routh critical value  $\mu_1$ . On the other hand if the sign of this term in the normal form is negative then for v = 0 the stable and unstable manifolds persists and then as v decreases from zero they detach from the equilibrium to follow a hyperbolic periodic solution.

#### On infinite beams simply supported

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This work provides sufficient conditions for the existence of solutions to fourth-order nonlinear ordinary differential equations with Lidstone-type boundary conditions on the real line. Using Green's functions, we formulate a modified integral equation and correspondent integral operators, which fixed points are solutions of the initial problem. Moreover it is proved that every solution of the Lidstone problem on the whole real line is an homoclinicsolution.

We consider an application to the bending of an infinite beam on poor soft soil, especially in coastal areas. This model considers a soil improvement by a strong granular layer, for fast drainage, supported by stone columns, and is used to consolidate the soft soil below the foundations of residential as well as industrial buildings, or to install railroads and roadways on soft soil or loose sands.

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# Entanglement and Pancharatnam phase of a Rydberg atoms system interacting with a quantized field

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# Abstract

We analyze the influence of the temperature and the number of halfwavelengths of the mode on the Pancharatnam phase and von Neumann entropy of a Rydberg atoms system interacting with a quantized field for different initial states of the system. Our results showed that the temperature and the number of half-wavelengths of the mode could be a control parameter for the Pancharatnam phase. Furthermore, a two-level atom in excited state interacting with a quantized field can be entangled by minimization the effect of temperature. On the other hand, when the system starts in a superposition state, the value of the information entropy increased significantly by increasing the temperature. Besides, the number of half-wavelengths of the mode has to be decreased to obtain the maximum value of the information entropy. This opens a new area for developing a Rydberg atoms system for future quantum computations and communication applications.

#### Numerical Modelling of Drug Delivery in an Isolated Solid Tumor

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Mathematical models and numerical methods are used due to their ability in predicting the cancer process. In the present study, the drug delivery in a solid tumor is investigated, numerically.

For the past 10 to 20 years, the main effort was to eliminate cancer cells. By recognizing the vital role of angiogenesis in tumor growth, much effort has been made to improve the antiangiogenic drugs [1]. Antiangiogenic drugs normalize the microvascular network and accordingly improve the drug delivery [2, 3]. The following equations were used to describe the fluid flow and solute transport in biological tissues,

$$-k\nabla^2 P_i = \frac{L_p S}{V} (P_B - P_i - \sigma_s (\pi_B - \pi_i))$$
<sup>(1)</sup>

$$\frac{\partial c}{\partial t} = D_{eff} \nabla^2 c - \nabla (\vec{v}c) + \frac{L_p S}{V} (P_B - P_i - \sigma_s (\pi_B - \pi_i))(1 - \sigma_f) C_p + \frac{PS}{V} (C_p - c) \frac{Pe}{e^{Pe} - 1}$$
(2)

The behavior of interstitial flow and solute transport is studied with respect to the different values of  $\alpha$ , in which  $\alpha$  shows the rate of transport across the vessel wall to the rate through interstitium [4]. Figure 1 shows the average non-dimensionalized concentration for different values of  $\alpha$  over time.

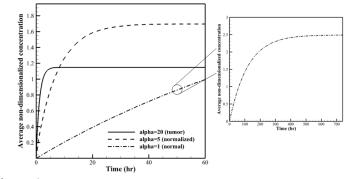


Figure 1: The average non-dimensionalized concentration over time.

Results show that the interstitial pressure gradient is created by normalization, which can cause fluid flow throughout the tumor. Due to the high permeability of the tumor, the concentration of the drug reaches its maximum value at the initial time after injection, while normalization can change this behavior as it is seen in figure 1. The concentration of drug increases by vascular normalization. Moreover, the concentration gradient is established by normalization that facilitates drug penetration into the inner parts of the tumor.

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# Investigation of the evolution of the microvascular network of a tumor under the inhibitory effect of Endostatin: A mathematical study

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Angiogenesis is the process of formation of new capillaries from the existing blood vessels in the vascular tumor growth phase. Folkman observed that when the new vessels are not formed, the tumor could not grow more than 2-3 mm. This phenomenon is due to angiogenesis and has established the basis of anti-angiogenesis treatment. In 1971, Folkman presented the concept of anti-angiogenesis in cancer treatment based on preventing the spread of vessels into the tumor [1, 2].

Mathematical models are used to study the angiogenesis since the 1970s. The angiogenesis was simulated in our previous works [3, 4] based on the initially proposed model of Anderson and Chaplain [5]. The model is in the discrete category, which can produce the morphology of microvascular network by simulating the motion of the endothelial cells. In present work, we developed our previous study by considering the inhibitory effect of Endostatin to investigate the anti-angiogenesis consequence on capillary network structure. Fig.1 shows the spatiotemporal evolution of the microvascular network with ten sprouts towards a linear tumor before and after anti-angiogenic treatment. Anti-angiogenesis makes the microvascular network sparser by pruning, as it is seen in Fig. 1. It is found that anti-angiogenesis normalizes the microvanter of the tumor. It is a useful method of cancer treatment especially in combination with other treatment methods such as chemotherapy.

Time(day)	2.5	5	7.5
Microvascular			
network evo-	0.8		
lution without	a6		
considering	× 0.5		
the anti-	as		
angiogenic	0.1		
drug	0 0.2 0.4 0.6 0.8 1		
Microvascular	6.9		
network evo-			Pruned
lution with			areas
considering	× as		
the anti-	e3		
angiogenic			
drug			

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### **Confidence Intervals for Regression Analysis of Taxi Trip Length**

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An interval of confidence is an important performance measure for any machine learning model, as the ability to determine a model's certainty of its predictions is incredibly valuable when making high stake decisions. In this study, we evaluate applications of machine learning algorithms, including Random Forest, Gradient Boosting, and Deep Learning Neural Networks on confidence intervals.

Different from deep learning using Artificial Neural Networks, Random Forest and Gradient Boosting are both ensemble algorithms which create many weak learners and aggregate the results to get a significantly more accurate prediction. With the multilayer perceptron, Monte Carlo Dropout techniques could be used to estimate the sample variance of Neural Networks. Similar techniques are applied to the "tree-based" algorithms by finding the variance of predictions made by many different trees. While these methods may be successful in finding an accurate range which the actual value falls into, these ranges are often very large and do not accurately convey how confident a prediction is. New methods are needed to develop accurate uncertainty measurements for Random Forest, Gradient Boosting, and Neural Networks.

We investigate the performance of the learning algorithms using NYC Taxi trip records from 2013 to predict the amount of time in seconds for each taxi ride. Considerations on feature selection, correlation and effect to the accuracy of predictions and the model's confidence are also discussed quantitatively.

# Absolute Bounds for the Number of Solutions of Certain Thue and Thue-Mahler Equations

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Let F(X,Y) be an irreducible binary form with integer coefficients of degree d > 2. Let *m* a positive integer. In 1909 it was demonstrated by Thue [1] that the equation

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

has only finitely many solutions in integers x and y. In 1991 it was conjectured by Stewart [2] that, in fact, the number of solutions to (1) in x, y coprime should not exceed some absolute constant, provided that m is sufficiently large. We provide evidence in support of Stewart's conjecture by proving the following.

**Theorem 1.** Let *n* be a positive integer such that  $\varphi(n) \ge 34$ , where  $\varphi$  is the Euler's totient function. Let *f* be the minimal polynomial of  $2\cos(2\pi/n)$  and  $F(X,Y) = Y^d f(X/Y)$  its homogenization, where  $d = \varphi(n)/2$ . Let *m* be a positive integer such that

$$p^k \mid m, \ p^k \ge m^{1/(2-16.2/d)}$$

for some prime *p* and positive integer *k*. Provided that *m* is sufficiently large, the number of solutions to (1) in *x*, *y* coprime is either 0, or 2 when  $4 \nmid n$ , or 4 when  $4 \mid n$ . If solutions exist, they are of the form (x,y), (-x,-y) if  $4 \nmid n$  and of the form (x,y), (-x,-y), (x,-y), (-x,y) if  $4 \mid n$ .

We will present Diophantine approximation techniques that enable us proving the above result, and explain how they can be further generalized to produce absolute bounds on the number of solutions (x, y, z) of a Thue-Mahler equation

$$|F(x,y)| = p^z$$

with *x*, *y* coprime,  $z \ge 1$ , and *F* as in Theorem 1.

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### BOLD.R: A software package to interface directly with BOLD through R

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The International Barcode of Life project (iBOL) continuously records and catalogs information acquired from samples collected by researchers and institutions around the world. The Barcode of Life Database system (BOLD) is the main workbench and mass storage system of the iBOL project. Advances in DNA barcoding and genetic analysis have resulted in a rapid increase in the volume of data stored on BOLD. Consequently, modern statistical techniques are playing an increasingly important role in the analysis of such extensive amounts of information. A popular software package for statistical analysis is R, however existing methods to retrieve data from BOLD into R are inconvenient, time-consuming or return limited information.

We developed an R library called BOLD.R which provides an accessible pathway to conveniently obtain data stored on BOLD directly into R. Users can access their own private data by using a secure login system provided through BOLD.R, or they can access public data without the need to login. All data obtained through BOLD.R is stored or cached with a consistent internal structure. This provides the user with the advantage of utilizing many existing libraries in R to analyze their data. BOLD.R is designed to complement existing packages, not compete with them. BOLD.R is also integrated with an assortment of functions which perform several common, useful tasks. An alpha version of BOLD.R was introduced during the International Barcode of Life Conference, 2017 and we aim to release a full version later this year (The alpha version can be downloaded at *http://boldsystems.org/BOLD.R*).

BOLD.R is a powerful, flexible convenient platform which provides the capacity to access and analyze large amounts of private and public data on BOLD directly through R. It can therefore become an invaluable tool which assists researchers make informed decisions in genetic barcoding, ecology, conservation, population genetics, evolutionary biology, bioinformatics and for education purposes as well.

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# **High-Order Error Control B-spline Gaussian Collocation Software for the Numerical Solution of PDEs**

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In this talk we discuss recent work associated with a family of high-quality error control software packages for the numerical solution of 1D partial differential equations. The packages employ adaptive B-spline Gaussian collocation for the spatial discretization and either Backward Differentiation Formulas or Runge-Kutta methods for the time integration. Both spatial and temporal discretizations are implemented using error control; the numerical solution is accepted only if the corresponding error estimates satisfy a user-defined tolerance. The more recent members of this family employ a pair of interpolation-based spatial error estimation schemes that significantly improve on the efficiency of the scheme used in earlier members of this family. We briefly review the underlying algorithms employed by the members of this family and provide numerical results showing the improved performance of the newest solvers. We also discuss extensions of this work to B-spline Gaussian collocation software for 2D PDEs.

# Calibration and Analysis of Structural Credit Risk Models with Occupation Time

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Credit risk is concerned with the probability of financial losses occurring due to changes in the credit quality of a firm. A rare occurrence of such sort is the *default event*, that often leads to bankruptcy proceedings, or liquidation, leading to large financial losses to both investors and speculators. In structural credit risk models, the asset level is compared to its liabilities at any time *t*, and the default event occurs when the asset level falls dangerously low compared to the liabilities.

In this talk, we study recently proposed structural credit risk model based on the occupation time [1, 2]. Assume that firm's asset value V(t) follows a geometric Brownian motion given by the SDE

$$dV(t) = rV(t)dt + \sigma V(t)dW(t).$$

The occupation time  $\mathcal{A}_t$  is defined as the time the process V has cumulatively spent below default barrier H:

$$\mathscr{A}_{t} = \int_{0}^{t} \mathbb{I}_{\{V(u) \le H(u)\}} du, \text{ where } H(t) = Ke^{-k(T-t)}, \text{ with } 0 \le t \le T, \quad k, K > 0.$$
(1)

The liquidation is triggered as soon as the occupation time  $\mathcal{A}_t$  exceeds a prespecified amount or the value V(t) has dropped below the liquidation barrier *L* given by

$$L(t) = Le^{-k(T-t)} \text{ with } 0 \le t \le T.$$
(2)

In this talk, we show how to compute the probability of liquidation and no-arbitrage prices of credit default swaps (CDS) and defaultable bonds. The calibration of the model parameters is done by the non-linear least squares method on CDS spreads available through Bloomberg. In the end, we compare the occupation-time models with other widely used structural models such as the Merton Model (1974) and the Black–Cox Model (1976).

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#### Game theoretical learning: performance guarantees for fictitious play

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This talk will discuss analytical results related to a game-theoretical learning algorithm known as *fictitious play*. Under this learning algorithm, each agent selects an action based on the assumption that other players are playing according to their historically-averaged strategy. After an appropriate time rescaling, this process can be described in mixed strategy space as a differential inclusion

$$\dot{x}_i \in BR_i(x),\tag{1}$$

where  $BR_i$  is the best response of the *i*th player, and x is the historical average of the strategies of all players.

These algorithms were originally proposed by economists to try to understand learning in game-theoretic settings. More recently it's been used by a variety of practitioners in engineering and data science as an algorithm to induce learning in complex, distributed, and multi-agent settings.

This talk will discuss recent analytical results which demonstrate that, in the context of potential or congestion games, these learning dynamics converge to reasonable pure strategy equilibria almost surely. These analytical results also provide convergence rate estimates, which guarantees robustness necessary for certain engineering applications. Time permitting, the talk will also discuss current work which extends and applies these results to games with adversarial players and to generative adversarial networks.

# Exact solutions and symmetry classification of heat equation on surfaces of revolution

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Eisenhart, in 1925, carried out a classification of surfaces of revolution according to their isometries. This work is devoted to investigate the question of the classification of surfaces of revolution according to the symmetries of heat equation. A complete classification is obtained and the minimal symmetry algebra is utilized to obtain the integral form solutions for the heat equation on any general surface of revolution. We also provide specific examples of exact solutions of heat equation on surfaces in different classes of classification including surfaces admitting only minimal symmetry algebra as well as surfaces admitting extra symmetries.

**Title**: First integrals and exact solutions of dynamical systems and dynamic optimization models.

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Abstract The notions of artificial Hamiltonian (partial Hamiltonian) operators are used to derive first integrals for first order systems of ordinary differential equations (ODEs) in epidemiology that need not to be derived from standard Hamiltonian approaches. We show that every system of first order ODEs can be cast into artificial Hamiltonian system  $\dot{q}^i = \frac{\partial H}{\partial p_i}$ ,  $\dot{p}^i =$  $\frac{\partial H}{\partial q_i} + \Gamma^i(t, q^i, p_i)$ . Moreover, the second order equations as well as system of second order ODEs can be written in the form of artificial Hamiltonian system. Then the partial Hamiltonian approach is employed to derive first integrals for systems under consideration. These first integrals are then utilized to find exact solutions of models from epidemiology for distinct class of population. For physical insight, the solution curves of closed-form expressions obtained are interpreted in order for readers to understand the disease dynamics in much deeper way. The effects of various pertinent parameters on the prognosis of the disease are observed and discussed briefly. Furthermore, we show that how one can utilize the partial Hamiltonian approach to compute the closed form solutions of some dynamic optimization growth models in the field of business and economics see e.g. Fisheries management and Vidale-Wolfe advertising models. This study provides a new way of solving the dynamical systems of first order ODEs, second order ODE, second order systems of ODEs as well as dynamic optimization models which are expressed into the artificial Hamiltonian system.

### Impact of influenza vaccine-modified effects on the outcomes of immunization

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Flu vaccines are designed to provide protection against flu infection and its complications. In a recent study of influenza vaccination, it is observed that viral shedding may be increased in vaccinated yet infected individuals [1]. In the first part of this talk, I will present the impact of influenza vaccination program on the infection risk of vaccinated and non-vaccinated individuals. Using the SIRV-type of disease transmission model, we study the balance between vaccine-modified susceptibility, infectivity and recovery needed in preventing an influenza outbreak, or in mitigating the health outcomes of the outbreak. To help informing vaccine manufacturers and individuals at high risks of developing serious flu-related complications, we assess the impact of vaccinating the population by different types of vaccines.

We show that, given an increase in pathogen shedding from vaccinated yet infected individuals, it is possible to observe a reduction in the total attack rate with increased vaccination uptake, even when the attack rates for both the vaccinated and non-vaccinated subpopulations are increased. By studying a relation between vaccine-modified effects at the epidemic threshold, we observe that a higher vaccination coverage and a lower basic reproduction number allows less strict vaccine-modified susceptibility and infectivity.

In the second part, I will talk about the estimation of vaccine-modified effects from the results of pre- and post-licensure studies.

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### Mathematical Results on Hyper-Inflationary Cosmological Model

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Recently, hyper-inflationary cosmological model has been proposed. In this model, the target manifold of scalar fields is a hyperbolic space which curvature is negative and slope of the potential does not affect accelerated expansion of the universe. It is interested in mathematical aspects of this model.

Since Penrose has proved a singularity theorem, which states that physically reasonable spacetimes are causally geodesic incomplete, three mathematical conjectures in classical general relativity has been proposed as follows. (1)Belinskii-Khalatnikov-Lifshitz (BKL) conjecture: Solutions to the Einstein equations should be asymptotically velocity-terms dominated (AVTD) ones near spacetime singularity. In other words, the evolution equations should become ODEs in time near spacetime singularity. (2)Cosmic no hair (CNH) conjecture: A solution of the Einstein-matter equations with a positive cosmological constant converges to the de Sitter solution at late times in a suitable sense. In particular, the solution is expected to homogenise and isotropise. (3)Strong cosmic censorship (SCC) conjecture: A solution of the Einstein-matter equations with a positive singularity, the solution at late times in a suitable sense. In particular, the global structure of spacetimes and are the most important open problems in mathematical general relativity. The aim of our research is to show the validity of the three conjectures by analyzing the Einstein equations with Gowdy symmetry in hyper-inflationary cosmological model.

We consider the following cosmological model. The Einstein-Hilbert action is

$$S = \int d^4x \sqrt{-g} \left[ R - g^{\mu\nu} G_{IJ} \partial_{\mu} \Psi^I \partial_{\nu} \Psi^J - 2V(\Psi) \right], \tag{1}$$

where g is a 4-dimensional Lorentzian spacetime metric, R is the Ricci scalar of the spacetime. The metric G of a target manifold for wave maps (scalar fields for hyper-inflation) is a hyperbolic metric with curvature length L (curvature is  $-L^{-2}$ ):

$$G = d\phi^2 + e^{\frac{2\phi}{L}} d\chi^2.$$
<sup>(2)</sup>

We assume that  $V = V(\phi)$  is a non-negative potential. Gowdy symmetric spacetimes describe spatially compact expanding universe. The metric of the Gowdy symmetric spacetimes with  $T^3$  spatial topology is given by

$$g = t^{-1/2} e^{\lambda/2} (-dt^2 + \alpha^{-1} d\theta^2) + t [e^P (dx + Qdy)^2 + e^{-P} dy^2],$$
(3)

where  $\lambda$ ,  $\alpha > 0$ , *P* and *Q* (gravitational fields) are functions of  $t \in (0, \infty)$  and  $\theta \in T^1$ . In this setting, Einsteinnonlinear scalar field equations become wave map. We prove a global existence theorem of solutions of the wave map equations and analyze asymptotic behavior of the solutions.

#### Numerical Integration of Stiff High-Index DAEs

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The DAETS solver by Nedialkov and Pryce [1, 2, 3] integrates numerically high-index DAE systems. This solver is based on explicit Taylor series and is efficient on non-stiff to mildly stiff problems, but can have severe stepsize restrictions on (very) stiff problems. Hermite-Obreschkoff (HO) methods can be viewed as a generalization of Taylor series methods. The former have smaller truncation error than the latter and can be A- or L- stable [4].

We develop an HO method for numerical solution of stiff high-index DAEs. As in DAETS, our method employs Pryce's structural analysis [5] to determine the constraints of the problem and to organize the computations of higher-order derivatives and their gradients. We discuss this method and its ingredients: finding a consistent initial point, computing an initial guess for Newton's method, automatic differentiation for constructing the needed Jacobians, and error estimation and control. We report numerical results on stiff DAE and ODE systems illustrating the performance of our method, and in particular, its ability to take large steps on stiff problems.

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# Lax-Wendroff schemes for quasi-exponential moment-closure approximations of kinetic models

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In many applications, the dynamics of gas and plasma can be accurately modeled using kinetic Boltzmann equations:

$$f_{,t} + \underline{v} \cdot f_{,\underline{x}} + \underline{F}(f) \cdot f_{,\underline{v}} = \frac{1}{\varepsilon} \mathbb{C}(f),$$
(1)

where  $f(t, \underline{x}, \underline{v}) : \mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^3 \mapsto \mathbb{R}^+$  is the probability density function (PDF) that describes the distribution of particles in phase space, t is time,  $\underline{x}$  is the spatial coordinate,  $\underline{v}$  is the velocity coordinate,  $\underline{F}(f)$  is the acceleration due to forces acting on the system (e.g., electromagnetic forcing due to interactions with the electromagnetic field),  $\mathbb{C}(f)$  is the collision operator, and  $\varepsilon$  is the non-dimensionalized mean-free path between collisions. This equation, along with equations describing the forcing ( $\underline{F}(f)$ ) and collisions ( $\mathbb{C}(f)$ ), represents an integro-differential systems posed in a high-dimensional phase space. If the system is sufficiently collisional ( $0 < \varepsilon \ll 1$ ), the kinetic equations may be replaced by a fluid approximation that is posed only in physical space. The precise form of the fluid approximation depends on the choice of the moment-closure. In general, finding a suitable robust moment-closure is still an open scientific problem.

In this work we consider a specific moment-closure based on a nonextensible entropy formulation. In particular, the true distribution is replaced by a Maxwellian distribution multiplied by a quasi-exponential function:

$$f \approx \beta_R \left(\underline{\alpha}\left(t,\underline{x}\right) \cdot \underline{\Phi}\left(\underline{v}\right)\right) := \frac{\rho\left(t,\underline{x}\right)}{\left(2\pi T\left(t,\underline{x}\right)\right)^{3/2}} \exp\left[-\frac{\|\underline{v}-\underline{u}\left(t,\underline{x}\right)\|^2}{2T\left(t,\underline{x}\right)}\right] \left[\max\left\{0,1+\frac{\underline{\alpha}\left(t,\underline{x}\right) \cdot \underline{\Phi}\left(\underline{v}\right)}{R}\right\}\right]^R, \quad (2)$$

where  $\rho(t,\underline{x}) : \mathbb{R}^+ \times \mathbb{R}^3 \mapsto \mathbb{R}^+$  is the mass density,  $\underline{u}(t,\underline{x}) : \mathbb{R}^+ \times \mathbb{R}^3 \mapsto \mathbb{R}^3$  is the macroscopic fluid velocity,  $T(t,\underline{x}) : \mathbb{R}^+ \times \mathbb{R}^3 \mapsto \mathbb{R}^+$  is the temperature, *R* is a globally constant integer chosen at the start of the simulation,  $\underline{\alpha}(t,\underline{x}) : \mathbb{R}^+ \times \mathbb{R}^3 \mapsto \mathbb{R}^M$  are parameters chosen to so that the first *M* moments of *f* and  $\beta_R$  match, and  $\underline{\Phi}(\underline{\nu}) : \mathbb{R}^3 \mapsto \mathbb{R}^M$  are the first *M* monomials in  $\underline{\nu}$ . We develop a high-order, locally-implicit, discontinuous Galerkin scheme to numerically solve resulting fluid equations. The numerical update is broken into two parts: (1) an update for the background Maxwellian distribution, and (2) an update for the non-Maxwellian corrections. We also develop limiters that guarantee that the inversion problem between moments of the distribution function and the parameters in the quasi-exponential function is well-posed.

# Recent results on Kolmogorov entropy compactness estimates for conservation laws

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Inspired by a question posed by Lax in 2002, in recent years it has received an increasing attention the study on the quantitative analysis of compactness for nonlinear PDEs. In this talk, I will present recent results on the sharp compactness estimates - in terms of Kolmogorov  $\varepsilon$ -entropy in L<sup>1</sup>- for hyperbolic conservation laws. Estimates of this type play a central roles in various areas of information theory and statistics as well as of ergodic and learning theory. In the present setting, this concept could provide a measure of the order of "resolution" of a numerical method for the corresponding equation.

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#### A debt management problem with bankruptcy risk and currency devaluation

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In this talk, a problem of optimal debt management is introduced which expands on the models derived in [2, 3, 1] and [4]. A debt repayment strategy is modeled as an interaction between a sovereign state and a pool of risk-neutral investors. At each time, the government decides which fraction of the gross domestic product must be used to repay the debt, and how much to devalue its currency. The total yearly income (GDP) of the borrower is governed by a stochastic process. When the debt-to-income ratio x(t) reaches a threshold  $x^*$ , bankruptcy instantly occurs. Moreover, we assume that the borrower may go bankrupt at a random time before the debt reaches  $x^*$ . We explore the derivation and analysis of the model through the lens of optimal control in infinite time horizon with exponential discount. The resulting stochastic control system depends not only on the present time t but on all future times. For a given bankruptcy threshold  $x^*$ , existence of an equilibrium solution is obtained by a topological argument. Our results show that the optimal control strategy does not use currency devaluation for debt values below a threshold.

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### A Probability Distribution for Discrete Quantum Walks on *n*-lines, *n*-cycles

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Classical random walks are the mathematical objects, known as a stochastic or random process, are proved to be a fundamental mathematical tool for modeling and simulating complex systems and natural phenomena. Among their various interesting applications, the development of stochastic algorithms is the paramount importance in computer science, telecommunication system, financial system, advanced DNA storage system, internet of things system, etc.

As a quantum analogue of classical random walks, in recent time quantum walks (QWs) have been well- studied processes. The same motivation as classical random walks, QWs are devised as the mathematical basis to develop sophisticated algorithms. Unlike random walks transformed by the probability transition matrices on the probability distribution, QWs are transformed by unitary revolutions. The probability distributions of quantum states are defined as the sum of squares of the norms of amplitudes. Due to the quantum interference effects, there exists a non-linearity map between the quantum state and the probability distribution. As a result, QWs have been shown to outperform random walks at certain computational tasks. Moreover, there exist both discrete and continuous QWs as the universal models of quantum computation. Both discrete and continuous QWs could be run on graphs, but their evolution is different. We use Schrodinger equation and Laplacian matrix for the time evolution of continuous QWs. On the other hand, the unitary operators which are applied in discrete time steps describe the time evolution of discrete QWs.

As for discrete QWs, an extra qubit register is defined to be the direction in which the walker unitarily moves from a node to its neighbor nodes. This model of QWs is called coin-driven QWs, is composed of two quantum systems: (1) a walker, which is a Hilbert space of finite or infinite Hp and (2) a coin, which is quantum system living in a two-dimensional Hilbert space Hc. Coin-driven QWs have been studied some detail by the scientific community such as the application to be perfect state transfer (PST) at [1], to do the teleportation at [2], many mathematical, statistical and computational properties remain to be discovered and explored [3]. In this research, we consider coin-driven QWs model based on the graphs where PST succeeds with certainty, namely *n*-lines, *n*-cycles. Firstly, the QWs based on *n*-lines and *n*-cycle are analyzed in detail where different cases of coin space are considered: Identity gate, Hadamard gate, Flip gate, and the special case of the imaginary complex number. In addition, the probability distribution and properties of underlying QWs have been barely explored.

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# A convergent numerical method for a multi-frequency inverse source problem in inhomogeneous media.

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Abstract: We propose a new numerical method to solve an inverse source problem for the Helmholtz equation in inhomogeneous media. This method reduces the original inverse problem to a boundary value problem for a coupled system of elliptic PDEs, in which the unknown source function is not involved. The Dirichlet boundary condition is given on the entire boundary of the domain of interest and the Neumann boundary condition is given on a part of this boundary. To solve this problem, the quasi-reversibility method is applied. Uniqueness and existence of the minimizer are proven. A new Carleman estimate is established. Next, the convergence of those minimizers to the exact solution is proven using that Carleman estimate. Results of numerical tests are presented.

#### **Fast Multipole Boundary Element Method for Thermal Radiation Problems**

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Study of multidimensional complex thermal radiation is always a challenging work in area of numerical heat transfer. Meanwhile, radiative heat transfer in semitransparent media is an important mode of heat transfer in such different areas of application as diffusion of neutrons, stellar atmospheres, optical tomography and so on. As a result, research on the radiative transfer problem has always been a very active and important area.

Mathematically, two types of models have been developed to describe the radiative heat transfer process. The first is the integro-differential radiative transfer equation (IDRTE) and the other is the radiative integral transfer equations (RITEs). Due to its strong nonlinearity, developing fast iterative algorithms is critical for computing the solution to IDRTE. Moreover, in the IDRTE model, the thermal radiation depends not only on the space variables but also on the angular variable which lives in a very high dimension space. This high dimensionality makes its approximation a very challenging task. On the other hand, the RITEs model is obtained by integrating the IDRTE model in the angular variable over all possible angles. As a result, the RITEs model is defined only in the space domain and it is angle free. This technique eliminates the high dimension difficulty at a cost of dealing with integral operators with singular kernels and with linear and nonlinear systems of dense matrices. In this talk, the boundedness of the four radiative integral operators is analyzed and proved theoretically. Based on these properties and the principle of contraction mapping, the existence and uniqueness of the solution to the integral system is proved [1].

The fast multipole method (FMM) was initially introduced by Rokhlin [2] as a fast solution method for integral equations, and then was further refined by Greengard [3, 4]. It can reduce the computational cost of matrix-vector multiplication from  $O(N^2)$  to O(N), which makes the computation of large-scale problems using boundary integral equation technique possible. The original FMM is highly efficient and yet quite cumbersome. For a general kernel, such as the radiative integral kernels in this paper, the analytic series expansion is difficult to find. So the original FMM is not easy to handle the more general integral equations. In recent years, some kernelindependent fast multipole methods (KIFMM) emerged such as [5, 6]. This talk focuses on the KIFMM in [5] only. The central idea of KIFMM [5] is to replace the analytic expansions and translations with equivalent density representations. It only requires the kernel evaluations and does not sacrifice the efficiency of the original FMM. It is found from numerical examples in [7] that the computational efficiency of the developed fast algorithm is much better than the conventional boundary element method.

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# **Epidemic dynamics and adaptive vaccination strategy :** scalar-renewal equation approach

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#### Abstract

We use analytical and numerical methods to investigate the adaptative vaccination strategy effects on the infectious disease dynamics in the closed population and in the demographically opened population. The methodology and key assumptions are based on Breda et al (2012). We show that the cumulative force of infection for the closed population and the endemic force of infection in the demographically opened population can be reduced significantly by combining two factors: the vaccine effectiveness and the vaccination rate. The impact of these factors on the force of infection can transform an endemic steady state into to a disease free state. Keywords: Force of infection, Cumulative force of infection, Scalar-renewal equation, Per capita rate of infectivity, Per capita death rate

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#### CONLEY-ZEHNDER INDEX AND APPLICATIONS WITH ELLIPTIC STABILITY FOR PERIODIC ORBITS.

#### DANIEL OFFIN

ABSTRACT. Roughly speaking, the Conley-Zehnder index measures the number of half windings of a fundamental solution for a periodic linear Hamiltonian system. This index, and its closely related cousin the Morse index for the equivariant action functional, can be used to give non perturbative arguments for linearized stability and instability for families of periodic orbits in Hamiltonian systems. Our first application to the Henon-Heielies Hamiltonian highlights the roll that mountain pass critical points of the action functional may play in the global dynamics of bound systems.

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### Liquid Surface Deformation due to Impinging Gas and Gas-Plasma Jets: Modelling and Experiments

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We consider liquid in a cylindrical beaker and study the deformation of its surface under the influence of an impinging gas jet that is generated by maintaining a constant gas flow rate from a stationary cylindrical tube with its axis coinciding with the axis of the beaker. Analyzing such a system not only is of fundamental theoretical interest, but also of industrial importance, e.g., in metallurgical, medical and environmental applications. The solution of the full set of governing equations is computationally expensive. Therefore, to obtain initial insight into relevant regimes and timescales of the system, we first derive a reduced-order model (a thin-film equation) based on the long-wave assumption and on appropriate decoupling the gas problem from that for the liquid and taking into account a disjoining pressure [1]. This is possible under suitable conditions, namely, when the liquid layer is thin and the typical liquid velocity is sufficiently smaller than that of the gas [2-4]. We also perform direct numerical simulations (DNS) of the full governing equations using two different approaches, the Computational Fluid Dynamics (CFD) package in COMSOL and the volume-of-fluid Gerris package. The DNS are used to validate the results for the thin-film equation and also to investigate the regimes that are beyond the range of validity of this equation (for example, when the liquid layer is thicker). We additionally compare the computational results with experiments. We find surprisingly that the thin-film equation produces good agreement with DNS and experiments even for flow conditions that are well beyond the theoretical region of the validity of this equation.

For a sufficiently thin film, we find that at relatively low gas flow rates, flow in the liquid evolves into a steady state with one recirculation region and with the interface having a cavity in the centre. At larger gas flow rates, the liquid film ruptures in the centre and dewets until reaching a steady state. We analyse the rupture time as well as the time evolution of the radius of the dry spot. For a thicker liquid layer, the flow in the liquid again evolves into a steady state at sufficiently small gas velocities. However, the number of the recirculation regions in the liquid increases as the liquid thickness increases. At higher gas flow rates, the flow in the liquid becomes unsteady with time-periodic or irregular oscillations being generated. We study the frequency and period of these oscillations and their dependence on the gas flow rate.

Finally, in addition to analysing gas jets acting on liquid surfaces, we also study gas plasma jets acting on liquid surfaces taking into account chemical kinetics. In particular, we analyse the accumulation and chemical reactions of plasma generated reactive species in the liquid and how these are affected by the flow in the liquid generated by the impinging jet. This has applications, for example, in water purification and wound treatment.

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### **Energy and Enstrophy Study of the Time Relaxation Model**

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In this presentation, we investigate energy and enstrophy conservations for a fluid model known as Time Relaxation Model, TRM. This filter based stabilization model with an added relaxation term is considered a high order fluid model (see Refs. [1, 2, 3]). Conservation of energy and enstrophy are two essential quantities characterizing change in the structure of the flow in time and are used to test if a simulation of a fluid flow is properly performed. Our research carries a study of these properties for TRM and provides a proof that these essential quantities, energy and enstrophy, are indeed conserved by this specific fluid model. In addition, it is shown that the energy and enstrophy obtained from TRM tend to the corresponding quantities of Navier-Stokes Equation, NSE, as the model parameters tend to zero. Our numerical experiments confirm the above conclusions.

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# Impact of Agricultural Tariffs and Trade Wars on Global Land Use

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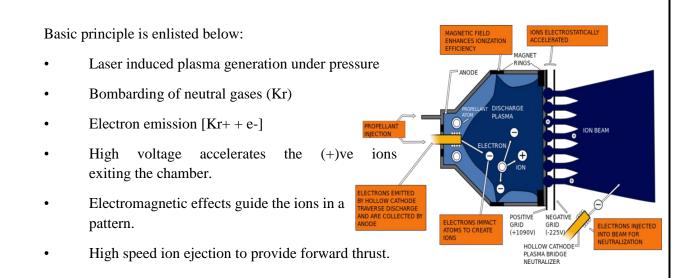
The ecological impact of land use changes by human dominated activities is massive. A significant portion of expanding anthropogenic land use is attributed to expanding croplands and pastures for food production. Earlier works have described increasing land-use as a socio-economic problem with complex human-nature coupling and identified drivers as well as inhibitors of farmland expansion at the cost of natural ecosystems. Our goal is to identify and study one socio-political driver of land-use expansion: trade-wars affecting the Agricultural Trade Network (ATN). The ATN plays a critical role inland-use problems as more than a quarter of agricultural land resources are accessed through trade. With recent declines in international trade deals in forms of trade-wars and tariff escalations, major shifts are expected in the structure of the ATN leading to unprecedented changes in global land-use. This leads us to our motivating question: what are the land-use impacts of trade wars? In our study we develop a dynamic network model to analyze the regional and global land-use outcomes of various scenarios of potential trade wars. Our model introduces direct functional relationships between percentage increase in tariffs, domestic supply-demand rates and effective land-use change under different scenarios of trade war between two nation states. Furthermore, we study the effects of different scenarios of implicit participation by non-participant countries in a trade war - i.e scenarios of countries filling in the import gap in the tariff imposing country. Results from our models suggest that all potential trade-war scenarios show significantly high global land-use changes in the order of millions of hectares of land. We also show that in most cases of agricultural trade war increase in number of implicitly participating nations causes increase in global land-use change by a significant factor. We also discuss cases where sharing the import gap in the tariff imposing country causes decrease in global land-use - a contradiction to the aforementioned result. We conclude by qualitatively comparing scenarios of potential trade-wars and identifying the trade-war scenarios with the worst fallout in terms of global land-use.

# CUBESAT PROPULSION SYSTEM VACCUM EXPANDED THERM - IONIC THRUSTERS

A *6U* - *CubeSat* is generally defined as a miniature satellite with a maximum weight of almost 6 Kg. To ensure the minimum weight factor, it is important that we implement lightweight materials with multi-functional capabilities for the manufacturing process.

*Graphene* is one of the lightest materials with excellent electrical, thermal and optical properties and high mechanical strength. Moreover, graphene ink can be used for printed electronics that consume less space, has more surface area for the thrusters. Due to viscosity and high surface tension, graphene ink is proven to be versatile enough to serve this purpose. *Lanthanum Hexaboride* and *Mylar polyester sheets* can be used for discharge tube fabrication and overall insulation purpose respectively.

It has been ages since the CubeSat propulsion techniques have only evolved and extended its domains. One of the most promising propulsion method is that of Ion thrusters. In our proposal, we present a *Laser Induced Thermionic Electron Emission System for CubeSat Propulsion*. Implementation of high energy laser sheets not only helps in weight reduction but also provides the optimum conditions for plasma formation.



For this system, we have planned a variable cross-sectional area design to make room for variable thrust operating conditions by means of pressure alterations which corresponds to the multiple speeds along the length of the tube and nozzle.

This setup apparently can eject ions at a speed over 30 km/s with significant contribution towards the forward thrust with *specific impulse ranging over 3000 seconds* which is considerably higher than the conventional propulsion techniques and subsequently consumes less power.

To increase the momentum of the exit ions further, a *vacuum annulus* can be used. The vacuum section not only increases the kinetic energy but also leads to ion expansion which corresponds to optimum pressure expansion.

In order to avoid overheating of the CubeSat, we propose the concept of *inter-surface refrigeration* by means of *Liquid Hydrogen* as a coolant.

This might revolutionize & replace the existing independent CubeSat propulsion systems in the near future.

# Algebraic Structure and Complexity of Bootstrap Percolation with External Inputs

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Bootstrap Percolation is a percolation process that is widely studied in statistical mechanics. It is an example of a boolean network on a lattice (or any other space) where the update rules are local and homogenous. The discrete dynamical system described by bootstrap percolation has a strictly monotonic behavior - that is, for any initial configuration of the system, the number of active nodes monotonically increases. Although bootstrap percolation is used in the mathematical modeling of some discrete event natural and artifical systems, [1] [2], the monotonic property of bootstrap percolation makes it non-ideal for the modelling of many natural systems which exhibit reversible or oscillatory behavior. Many non-monotonic variants of the bootstrap percolation model have been studied based on their context of application [3] [4]. In this paper we introduce a non-monotonic variant of the bootstrap percolation model called bootstrap percolation with external inputs. The model is introduced as a modification to the trade network model presented in [4]. The modifications address the drawbacks and assumptions of the model and present a more robust representation of cascades in international trade networks. In this paper we study the hierarchical algebraic structure and the complexity of the discrete dynamical system defined by our model. We represent our discrete dynamical system as a transformation semigroup (automata) and use the Krohn-Rhodes theorem of semigroup decomposition to study the algebraic structure and complexity of our system. The complexity measure we use provides qualitative insights into existence of pools of reversibility in our dynamical system - a higher complexity indicating more levels of reversible loops (or equivalently, transformation groups) in the Krohn-Rhodes decomposition of our system. We demonstrate how the structure and complexity of our model transformation semigroup varies with changes in model parameters, network structure and discuss the implications of these variations on our model of cascades in international trade network.

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### Fairness Comparisons of Strategyproof and Efficient Matching Rules

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We study one-to-one matching models where agents have strict preferences over objects and objects have strict priorities over agents. The main objective is to determine which matching rules are more fair than others among strategyproof and efficient matching rules, based on the given priorities of objects. We examine two natural definitions that allow for comparing matching rules in terms of object priority violations, known as *justified envy*:

1. A rule **JE-dominates** another rule if it has no justified envy at any preference profile where the other one has no justified envy, and there is at least one additional preference profile at which the dominating rule has no justified envy, while the dominated one has.

2. A rule **cardinally JE-dominates** another rule if the number of justified envy instances are either the same or lower at each preference profile for the dominating rule, and there is at least one preference profile with a lower number of justified envy instances.

Using these criteria, we demonstrate that when the object priorities are not acyclic the TTC does not stand out as the unique most fair strategyproof and efficient matching rule, contrary to some indications in the literature ([1, 4]). Specifically, we prove the following results.

**Theorem 1.** There is no unique strategyproof and efficient matching rule that either JE-dominates or cardinaly JE-dominates all other strategyproof and efficient matching rules for an arbitrary cyclic priority profile, where a priority profile is **cyclic** if it is not acyclic in the sense of [2] and [3].

*Note:* For an acyclic priority profile, the TTC is the unique rule that both JE-dominates and cardinally JE-dominates any other strategyproof and efficient matching rule. This is well-known, since in this case the TTC rule coincides with the Gale-Shapley Deferred Acceptance rule which is fair (i.e., has no justified envy at any preference profile).

**Theorem 2.** For an arbitrary priority profile, the TTC rule is neither JE-dominated nor cardinally JE-dominated by any other strategyproof and efficient matching rule.

**Theorem 3.** If the priority profile is **strongly cyclic** (satisfies an intuitive stronger notion of cyclicity), there is no strategyproof and efficient matching rule that either JE-dominates or cardinally JE-dominates another strategyproof and efficient matching rule.

In sum, our results suggest that the more cyclic the priority profile, the less likely it is that we can compare strategyproof and efficient matching rules in terms of basic fairness criteria, and therefore the less prominent TTC becomes as a relatively fair rule.

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#### **Exploring the Fractional Derivatives of the Riemann Zeta Function**

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The Riemann zeta function  $\zeta(s)$  and its derivatives  $\zeta^{(k)}(s)$  are given by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$$
 and  $\zeta^{(k)}(s) = (-1)^k \sum_{n=2}^{\infty} \frac{(\log n)^k}{n^s}$ 

for all natural numbers k, everywhere in the half-plane  $\Re(s) > 1$ . Each of them can, by a process of analytic continuation, be extended to a meromorphic function with a single pole at s = 1.

In 2003, Skorkhodov [7] observed that discretely increasing k moves the non-trivial zeros of  $\zeta^{(k)}(s)$ , in a one-to-one fashion, to the right. Investigating the zero-free regions of higher derivatives  $\zeta^{(k)}(s)$  in [1] the authors proved this phenomenon for sufficiently large k, and found that there these derivatives have *identical* zero counts. Numerical results suggest that these sequences of zeros continue on the left half plane and also contain the zeros of derivatives on the negative real axis [2].

The existence of a visible "flow" of the zeros suggests that perhaps an in depth study of the *fractional* derivatives could provide a missing link needed to establish this fascinating but currently little-understood property. We have found that, among the multitude of existing definitions of fractional derivatives, the reverse Grünwald-Letnikov derivative works best for situations dealing with  $\zeta(s)$  and its derivatives. In fact, in [3] we have applied it successfully in a proof of a conjecture by Kreminski [6].

Computations suggest that the sequences of zeros of the integral derivatives lie on the curves  $\zeta^{(\alpha)}(s(\alpha)) = 0$ where  $\alpha$  is a positive real number. While many observations are not proven yet, just as in the case of integral derivatives the disk |s-1| < 1 the fractional derivatives of  $\zeta(s)$  are zero free [4]. We report on our numerical explorations of the fractional derivatives of the Riemann zeta function and first results, including the generalization of the vertical zero free regions from [1] to fractional derivatives.

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# New families of relative equilibria in the curved N-body problem

Ernesto Pérez-Chavela Juan M. Sánchez-Cerritos

#### Abstract

The curved two dimensional N-body problem, is a generalization of the classical planar Newtonian N-body problem to spaces with constant curvature.

In this talk, we consider 5 and 7 positive point masses located symmetrically on the same geodesic (collinear configuration). Given a fix configuration, we show if there are or not masses which generate a relative equilibrium with such configuration. Given positions for which relative equilibria does exist, there are infinitely many values of masses which generate such solutions.

#### Early-warning signals of epidemics in a multiplex disease-behaviour model

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Resurgences of vaccine-preventable diseases in many countries have overwhelmed public health systems, interrupted tourism and public services and decreased GDP through the huge costs of large-scale interventions [1]. These events have been driven by falling vaccination rates [2]; this is due to the spread of vaccine distrust, facilitated by the ease of spreading questionable content on social networks [3]. This, combined with users' explicit ability to choose their social contacts on these networks, makes it difficult to effect any mass changes in sentiment beneficial to public health.

The negative effects of these outbreaks can be mitigated through the use of predictive tools to coordinate preventative interventions. This close relationship between social and disease dynamics suggests that patterns of social interaction may be used to predict these epidemics [4]. Early-warning signals, easily recognisable and statistically significant behaviours that precede phase transitions in physical systems, have shown promise as methods for quantifying these predictions [5].

A multiplex agent-based simulation was used to model the spread of a vaccine-preventable disease in a randomly networked population with different initial proportions of vaccinators. Parameters representing the imposition of social norms and the perceived risk of vaccination were varied, with nodes reevaluating their vaccine sentiment upon social interaction with dissenting contacts.

Results yielded various metrics such as join count statistics and spatial autocorrelation coefficients, that predicted epidemics through monitoring the connectivity of the social network and synchronisation of network dynamics. This work makes a unique contribution to the current literature surrounding coupled disease-behaviour systems and early-warning signals, and will provide a basis for future work in the area.

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#### Approximate Bayesian Computation for the Distributions of Wealth and Income

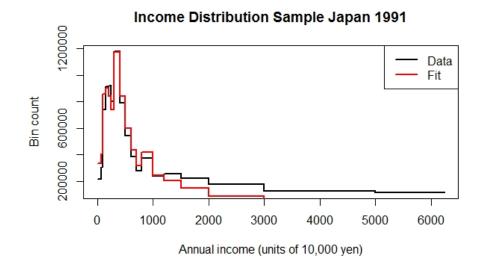
Z. Nan<sup>1</sup>, L. Pichl<sup>1</sup>, T. Kaizoji<sup>1</sup>, E. Scalas<sup>2</sup>

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We study the inequality in the distributions of wealth and income, as it evolves over the past 3 decades, focusing on trends in open government data from Japan and the UK. The generalized beta distribution is used as a theoretical model with the probability density function given by

$$p(x;a,b,c,p,q) = \begin{cases} \frac{|a|x^{ap-1}(1-(1-c)(x/b)^a)^{q-1}}{b^{ap}B(p,q)(1+c(x/b)^a)^{p+q}} & \text{for } 0 < x < \frac{b}{(1-c)^{1/a}} \\ 0 & \text{otherwise} \end{cases}$$

where x is the value of the stochastic variable and a, b, c, p and q are parameters (all non-negative in the present case). The symbol B(p,q) stands for the beta function. We have developed several numerical procedures to fit the above distribution to the actual data, which are partitioned in un-evenly sized income/wealth bins within the range of  $(0,\mu)$ , where  $\mu$  denotes the maximum value reported in the data set. We can simulate the entire population sample at the order of several million individuals to optimize the data fit. The figure below shows an example for the income distribution of Japan in 1991 as reported in open government data by Japan's Ministry of Finance. It



can be seen that the fit works well for low-to-mid range incomes, where most data belong, and has the tendency to underestimate high income groups. At the conference, we will report a systematic analysis for the Japan's time series of income data, including the Lorenz curve and Gini index, and discuss the long tail behavior [1].

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### Weighted representative democracy

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Existing systems of representative democracy fall into two broad classes: *regional representation* (used in Canada, the United States, and the U.K.) and *proportional representation* (used in many European countries). Both of these systems have serious disadvantages. We propose a new system of democratic representation. In our proposed system, any voter can choose any legislator as her representative; thus, different legislators can represent different numbers of voters. Decisions in the legislature are made by *weighted voting*, where the weight of each legislator is determined both by the number of voters she represents, and the level of confidence that each of these voters expresses in her judgement. We show that, if the size of the electorate is very large, then with very high probability, the decisions obtained in the legislature agree with those which would have been reached by a popular referendum. Thus, the legislature does a good job of expressing the popular will. We obtain this asymptotic result for several classes of voting rules:

- Simple majority vote between two alternatives.
- Arrovian preference aggregation rules which use only *majority tournament* data (e.g. the Copeland rule and the Slater rule).
- Arrovian preference aggregation rules which use only *majority margin* data (e.g. the Borda rule and the Kemeny rule).
- Judgement aggregation rules corresponding to majority tournament and majority margin rules (e.g. the generalized Slater rule and the median rule).

The V International AMIMCS Interdisciplinary Conference Waterloo, Ontario, Canada [August 18-23, 2019]

# Simulating a Classical Swine Fever Introduction into Commercial Pig Farms in Ontario

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Foreign animal diseases of swine are of significant concern for Ontario swine farmers. In the absence of such diseases, computer simulation models can help us examine disease outbreak scenarios. The objective of this study was to simulate the introduction of classical swine fever (CSF) into Ontario swine farms and test the efficacy of known interventions.

We used a previously developed synthetic swine population comprised of six production types. Both direct and local (proximity based) transmission were considered. Three intervention scenarios were assessed for 1-year period, a) low-intensity: immediate depopulation within 500 meters of an infected farm, movement restriction and post-outbreak surveillance (3-km), and low-intensity traceback, b) moderate-intensity: immediate depopulation (5-km), movement restriction and post-outbreak surveillance (5-km) and moderate-intensity traceback, c) high-intensity: immediate depopulation within 1-km radius, live attenuated vaccination (1-km), movement restriction and post-outbreak surveillance (10-km) and high-intensity traceback.

The average number of newly infected farms were somewhat lower within the high-intensity intervention scenario (high-intensity (mean (95% confidence interval (CI)) – 455 farms (95% CI: 444 -446), moderate-intensity – 510 farms (95% CI: 501 – 520), low-intensity – 577 (569 – 586)). Regardless of the intervention intensity, 18%-23% of the farms were infected.

Regardless of intervention intensity, the models suggest that a large proportion of pig farms in Ontario could be infected if CSF virus is introduced to the population given the parameter value estimates. However, a better understanding of the contact between farms and the current baseline disease detection probability could help us develop more accurate simulation models.

# A symplectic sightseeing tour on singular Hamiltonian systems

#### A. Portaluri

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Is the solar system stable? This is maybe one of the oldest open question in dynamical systems. It is still a lively and very active research field starting from Newton, Lagrange, Maxwell, Poincaré, Birkhoff (only for mention few of them) who proved several astonishing results in this direction. A lot of useful techniques to tackle this problem, were developed during the last decades, e.g. symplectic and contact methods, equivariant variational critical point and index theory!

In this talk we introduce some new ideas behind many recent results on this topic and we discuss some new perspectives and challenges on singular (weak force) Lagrangian problems. We discuss some recent (in)stability results for a plethora of periodic motions via symplectic techniques.

# Error estimates for a finite volume method for the Laplacian on spherical icosahedral grids

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This work derives supra-convergence phenomena of the discretization of the Laplace's equation on spherical icosahedral geodesic grids. First, we introduce the properties of the continuous problem on the sphere  $\mathbb{S}^2$ . We outline geometric characteristics to generate spherical icosahedral geodesic grids by recursive refinement. In particular, we define a discretization of the Laplacian by Finite Volume Method. In fact, we present the feature of the truncation error via some numerical examples. Finally, we show that usual error estimates of the approximate solution are of quadratic order when the spherical icosahedral geodesic grid used.

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#### **Reversible Image Reconstruction for Reversible Data Hiding in Encrypted Images**

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Recently, reversible data hiding in encrypted image (RDHEI) [1-2] has become a hot topic. RDHEI can protect the privacy of the original image content by encryption and enable data hider to manage the encrypted image by reversible embedding additional data. In this abstract, we aim to propose a new scheme for RDHEI, which is based on reversible image reconstruction (RIR). RIR rearranges the original image to construct a redundancy image and makes the meaningful information in the original image invisible, so this rearranged image can be used as the encrypted image. To ensure safety, the statistical characteristics of the rearranged image will be different from that of the original image.

The process of RIR is shown in Fig. 1. As we can see, RIR contains three steps. The first step contains two phases: the first-order rearrangement and local smoothness adjustment (LSA). The first-order rearrangement will try to make the whole image pixel distributed from small to large, and LSA adjusts the smoothness extent of small regions.  $\eta$  is the parameter of smoothness ratio, which is the ratio of the smoothness of R''(I) to the smoothness of *I*. The cycle of LSA will end until  $\eta$  meets the end condition that is  $\eta$  is less than 1.3. The second step of RIR compresses the generated accessorial data (A and B), merges them into a sequence, and encrypts the sequence to enhance the security. In the last step, the processed accessorial data will be embedded into R'''(I) to generate the encrypted image E(I). The recovery process of RIR is the inverse process of Fig. 1.

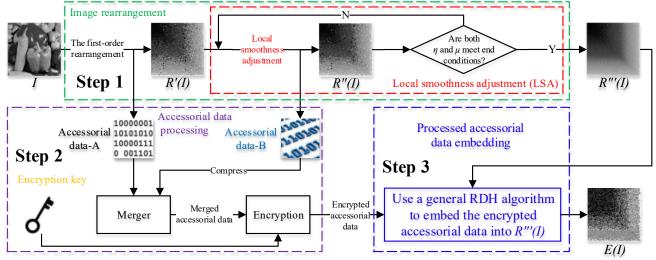


Fig. 1 The process of redundancy space construction.

As E(I) contains redundancy, general reversible data hiding method for plain image can be employed to embed additional data into it. Depending on the reversible data hiding method used, the receiver side operations in the RIR based RDHEI scheme can be separable or inseparable. Experimental results show that the performance of the proposed RIR based RDHEI scheme outperforms the previous RDHEI algorithms.

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# A mathematical model for studying the impact of education campaigns on the HIV/AIDS transmission.

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In this work, a mathematical model based on the ordinary differential equations is used for evaluating the impact of the education campaigns on the HIV/AIDS transmission. The model takes into account educated persons and uneducated persons. Using the data coming from the literature review, we computed the basic reproduction number  $R_0$  representing the average number of new infection generated by a single HIV/AIDS infection person in a susceptible population and we studied the evolution of  $R_0$  as the function of the rate of susceptible educated persons and the rate of infected educated persons. Results show that after education campaigns, there is a decreasing in term of the number of infection cases. Public education campaigns change behaviors of infected persons and modified the force of infection considered as a great parameter used by the model. The developed model could help to plan strategies to predict the number of infected cases in the short and long term. **Keywords.** HIV/AIDS, Mathematical modeling, education campaigns, basic reproduction rate

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#### Computational topology in neuroscience

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Functional magnetic resonance imaging (fMRI) is a technique that plays an important role in brain imaging analysis. After thresholding the blood-oxygen-level-dependent (BOLD) contrast image, its excursion set is shown to have a close relationship with the activated brain region ([1]). Recently, research has focused on using more topological information into fMRI analysis. Some topological invariants of excursion sets are proposed to be descriptive features of brain images. In supervised classification, [2] evaluates the performance of the Euler characteristic (EC) of excursion sets as a descriptive feature for 2 or 3-dimensional objects. The EC of the excursion set also contributes to threshold decisions for the detection of activated regions ([3]). Particularly in scalar-on-image regression, [4] develops a class of Bayes nonparametric models by thresholding a smooth Gaussian prior. The number of connected components of the excursion set is then studied for statistical inference. Since these images, or 3-dimensional objects, are modeled by smooth Gaussian random fields, theorists are interested in the distributions of topological invariants of excursion sets with regularity. We will introduce some known applications and results related to the EC and the number of connected components of excursion sets for smooth Gaussian random fields.

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# Applied Machine Learning to Define and Predict Pain Volatility in Users of the Manage My Pain App

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Measuring and predicting pain volatility (fluctuation or variability in pain scores over time) can help improve pain management. Perceptions of pain and its consequent disabling effects are often heightened under conditions of greater uncertainty and unpredictability. Pain volatility contributes to such uncertainty and unpredictability. This study aimed to apply machine learning methods to (1) define a new measure of pain volatility and (2) predict future pain volatility levels at the sixth month of app use from users of the pain management app, Manage My Pain, based on demographic, clinical, and the first month's app use features.

Users with at least five pain records in both the first and the sixth months (N=879) were included in this study. Pain volatility was defined as the mean of absolute changes between two consecutive self-reported pain severity scores (0-10 numeric rating scale) within the observation periods. The k-means clustering algorithm was applied to users' pain volatility scores to establish the threshold for discriminating low from high volatility. Thus, users were divided into two classes based on their pain volatility scores at the sixth month: low volatility (n=694) and high volatility (n=185). Subsequently, 130 demographic, clinical, and app usage features were extracted from the first month of app use to predict these two volatility classes at the sixth month of app use. Prediction models were developed using four machine learning methods: (1) logistic regression with ridge estimators; (2) logistic regression with Least Absolute Shrinkage and Selection Operator; (3) Random Forests; and (4) Support Vector Machines (SVM). Training and testing were conducted using the 5-fold cross validation method. Accuracy for both low and high volatility classes was calculated to compare the performance of the prediction models. The class imbalance issue was addressed by multiple random under-sampling of the majority class (low volatility) in the training dataset. Prediction results from the models trained on these random subsamples were consolidated using majority voting. Results show that Random Forests performs the best among the four machine learning methods as it achieves approximately 70% accuracy for both classes. Two different feature selection methods were applied: mean decreased Gini impurity and gradual removal of features based on the information gain criterion in Random Forests-based prediction models. Nine out of 130 features were selected that we consistently identified to be highly predictive by both methods across all testing sets. Random Forests achieved approximately 68% prediction accuracy for both low and high volatility classes using these nine features.

This is the first study of its kind to define and predict chronic pain volatility using machine learning methods. The study involves the use of a large dataset based on real-world data from people with pain who autonomously use the app. Results from this study show that by using features of the dataset extracted over a onemonth period, pain volatility six months later can be predicted, with a reasonably high degree of accuracy.

# Modeling the gastrointestinal pathway of *L. monocytogenes* and the role of host factors on the survival of the pathogen

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We develop an agent-based gastric simulator for a human host to illustrate the within- host survival mechanism of *L. monocytogenes*. The model incorporates the gastric physiology and digestion process that are critical for pathogen survivals in the stomach. Mathematical formulations for pH dynamics, stomach emptying time, survival probability in terms of gastric acid are integrated into the model to evaluate the gastric survival of ingested pathogens. Model parameters are estimated by using in vitro data relevant to human stomach and *L. monocytogenes*. In the absence of extensive scientific experiments, that are not feasible on the ground of ethical and safety concerns, this model may provide a supplementary tool to evaluate the pathogen survivals and subsequent infections in the host.

### From Neural Integration to a Statistical Model: Skellam Process with Resetting

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Point processes are common in modelling and analysis of neural spike trains, however, the literature is, as yet, not as researched on multivariate versions of such processes. With the current technologies in simultaneous recordings of multiple neurons, the need for computationally efficient and scalable multivariate point processes is eminent. We discuss the shortcomings of the commonly-used Poisson process and its limited multivariate versions. We then introduce the relatively new and flexible alternative; Skellam process with Resetting (SPR) [1]. Motivated by the process of neural integration, the SPR model is biologically justified, and has flexible multivariate generalization, allowing for a full range of correlation structure to model synchronous/ asynchronous spiking activities. This flexible correlation structure is particularly important as inhibitory and excitatory synapses both exist across brain areas. The SPR model is defined as a modified version of the difference between two independent Poisson processes, where the modification adjusts the stochastic process for neural refractoriness. In its multivariate version , including a third common Skellam term allows for flexible correlation structure [2]. Conditioning on the common term (marginal estimation), fitting the multivariate SPR model can be done using efficient parallel computation, hence addressing a common challenge in the analysis of multiple spike trains within a point process framework. Although SPR is a model for data (not for the brain), we show that it differentiates between experimental conditions in a decision-making experiment involving the prefrontal cortex.

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# **Gap Avoidance Conditions in Optimal Control**

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In relation with certain domain extensions of optimal control problems –like convex relaxation or impulsive, space-time, embedding of unbounded control problems– the *normality* of an extended optimal extremal has been shown to be sufficient for the avoidance of a *infimum gap*, the latter meaning a stricly negative difference between the infimum of the extended problem and the infimum of the original problem. We prove that, far from being a peculiarity of those specific extensions, this sufficiency turns out to be a universal cryterium, provided the original family  $\mathcal{V}$  of controls is *abundant* in the extended family  $\mathcal{W}$ . *Abundantness*, which is stronger than the mere  $C^0$ -density of the original trajectories in the set of extended trajectories, is a dynamical-topological notion introduced by J.Warga, to whom a first result of this kind is due.

# Fractional calculus approach for the phase dynamics of Josephson junction under the influence of magnetic field

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Superconductors have widespread applications in modern technology. Two superconductors when weakly connected, for example by a very thin non superconducting barrier, a current flows through the barrier without any dissipation of energy and power supply [1, 2]. This phenomenon is called Josephson Effect and the junction is called Josephson Junction. A wide range of modern day technologies operate using this phenomenon. Superconducting quantum interference devices (SQUIDs) and Superconducting tunnel junction detectors (STJs) are based on Josephson Effect [2, 3]. This article presents the phase dynamics of a long Josephson junction in voltage state under the influence of constant external magnetic field. Fractional calculus approach is used to model the evolution of the phase difference between the macroscopic wave functions of two superconductors across the junction. The governing non-linear fractional partial differential equation is then solved using finite difference-finite element scheme [4]. In order to validate the developed numerical scheme, a numerical error analysis of the scheme has been performed and compared to the postulated theoretical error estimates. The physical quantities of interest like Josephson current density and voltage across the junction have been computed. The effects of various parameters in the model on the phase difference, Josephson current density and voltage are analysed graphically with the help of numerical simulations.

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# An experimental and numerical study verifying the effects of spectral enrichment due to nonlinear wave propagation in trumpets and trombones

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In 1996, Hirschberg *et al.* published experimental findings indicating that shock waves formed in the trombone under certain playing conditions [1]. The production of shock waves is dependent on the input pressure, the length of the bore [1] and the corresponding geometry prior to the bell [2]. The consequences of wave steepening is referred to as *spectral enrichment*, and is characterized as the transfer of sound energy from the lower to higher spectral components [4]. Moreover, the harmonic content of a note is responsible for producing a specific timber (quality of sound) [1], [3].

In this paper, we present our own experimental findings and analysis for both the trumpet and trombone to verify the claims made in the literature about spectral enrichment. In addition, the shock distance expression presented in [1] is used to calculate whether it is theoretically possible for shock waves to form within the length of our instruments for the notes we measured in the lab. Finally, equations of motions found in gasdynamics are used to model the nonlinear wave propagation within the bore of the trumpet and trombone for the loudly measured  $B_3^b$  notes. Simulations are carried out in three-dimensions where the cross-sectional area of the tubing, including the shape near the mouthpiece-shank, is properly modelled. The equations of motion are numerically solved using the Discontinuous Galerkin method. Our numerical results are reviewed to determine whether weak shocks were produced within the computational instruments.

Our experimental and numerically findings indicate that for the particular notes measured in the lab, weak shocks form within the trombone. For the trumpet however, only wave steepening is observed. These results also agree with the calculated shock distance for the  $B_3^b$  notes.

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#### On the Problem of Maximum Delay Margin in Linear Control

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Time delays are ubiquitous in linear time invariant (LTI) systems, especially in networks, and may occur through communication delay, computational delay or physical transport delay. Consequently, systems with delay have been the subject of much study in systems and control. Given an unstable (LTI) system with time delay, in this talk we consider the problem of finding the largest time delay  $\tau_{max}$  such that there exists an LTI controller that stabilizes the time delay system for each delay in the interval  $[0, \tau_{max}]$ . This delay margin problem is related to the gain margin and phase margin problems in robust control, but the delay margin problem is more complicated, and many unsolved problems remain.

This talk is based on results first presented in [1] and builds on the approach in [2], [3], which formulates a sufficient condition for the maximum delay margin in terms of an interpolation problem with a real weight and obtains a lower bound using a rational approximation of the weight. In [1] we instead reformulate the interpolation problem as an infinite dimensional analytic interpolation problem and solve it directly using techniques from function theory and complex analysis. Furthermore, we introduce a constant shift in the domain of the interpolation problem. In this way we are able to improve on their lower bound for the maximum delay margin, and in numerical examples we can in some cases come (arbitrarily) close to the true upper bound.

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### Distance between shapes for closed polygonal curves

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This paper describes an extension of previous work on Local Indicators of Space and Shape Association (LIS-ShAs) [1] to include closed polygonal curves. The previous work applied to open polygonal curves and used a variation of local Geary's C SA measure with the Fréchet distance to define the neighbourhood structure and the Small-Le metric to define distance between attributes - in this case the attribute is an invariant representation of feature shape. In the case of closed polygonal curves, there is no canonical choice for starting and ending vertices for the polygonal curve so the methodology developed for open curves can not be directly applied. This paper introduces two new techniques to allow closed curves to be considered.

The first approach finds the minimum distance from the set Small-Le distances calculated from cyclical permutation of the closed curve's vertices (this is linear in the number of vertices). The second approach introduces a recursive coding based on Kendall coordinates and a new triangle-chain representation. A case study of both techniques and discussion of results is provided.

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# Thermal Conductances of Silicon Phononic Crystals Determined by Reverse Non-Equilibrium Molecular Dynamics Simulations

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Phononic crystals are periodically structured, synthetic materials designed to control the propagation of elastic waves. The periodic structuring opens the door to custom tailoring of the dispersion relations of elastic waves and enables the creation of vibrational band gaps (forbidden frequency ranges) in the material. Phononic crystals have numerous potential applications in areas such as noise control, ultrasound imaging and telecommunication. In non-metallic materials lattice vibrations are the principal mechanism of heat transport. For this reason, nanoscale phononic crystals with operating frequencies in the THz regime can be utilized to control the flow of heat. This is interesting for energy harvesting and novel heating or cooling technologies.

In this work, phononic crystals made from silicon nanoparticles and nanowires are studied with molecular dynamics simulations. For the determination of thermal conductances, we employ Reverse Non-Equilibrium Molecular Dynamics (RNEMD) [1] which — despite some drawbacks — is a straightforward way to determine the thermal conductances from molecular dynamics simulations. It is known that the thermal conductance of short nanowires deviates from the linear length dependence observed on the macroscale [2]. For this reason, we calculate the thermal conductance of phononic crystals of different length and compare the results with similar nanowires. In addition to this, we present results showing the influence of grain boundaries and the presence of band gaps on the thermal conductance.

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#### Stochastic simulations for reactive and diffusive systems

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Diffusion plays a direct and indirect role in a vast number of biological and chemical processes. Partial differential equations are often used to model the direct role of diffusion in systems that have spatial inhomogeneities, while indirect contributions might be the use of diffusion-dependent reaction rates in well-mixed chemically reactive systems. Stochastic noise can lead to interesting changes that traditional ordinary differential equations (ODEs) in the form of reactive rate laws, or partial-differential equations (PDEs) in the form of reaction-diffusion equations, are not capable of predicting. Stochastic simulations have found great utility in their ability to model behaviour that is not possible to predict with ODEs or PDEs, thus effectively modeling behaviour that is exhibited by systems for which ODE and PDE models no longer apply.

Stochastic simulation methods have gained much popularity since the original work by Gillespie [1]. This particular method is commonly referred to as Gillespie's algorithm, or as SSA (Stochastic Simulation Algorithm). Spatially extended models incorporating direct effects of diffusion with an a priori value for the diffusion coefficient can be modeled using an extension thereof called the ISSA (Inhomogeneous Stochastic Simulation Algorithm). Various related methods to overcome the numerical and theoretical limitations of these approaches, as well as to improve overall efficiency, have been introduced in the literature thereafter. A recent overview can be found in [2]. More detailed, particle-based stochastic algorithms have gained more recent attention, and include Brownian dynamics (BD) simulations, as well as Multi-particle collision dynamics (MPC). BD can be coupled to reactions to create a more detailed, microscopic model of the system, as well as MPC, the latter being referred to as Reactive MPC (RMPC) in the literature. In contrast to BD, RMPC is more detailed in nature, and can additionally be used to not only model the dynamics of a reaction-diffusion equation in one limiting case, but also to model fluid dynamics behaviour including incorporation of slip and no-slip boundary conditions. This latter effect is challenging to incorporate in BD or ISSA approaches.

The focus of this talk is to highlight recent advances in stochastic simulations for reactive and diffusive systems using RMPC. The RMPC mechanism will be explained, and simulation results for a number of reaction-diffusion systems will be presented, including the chemotactic response of an E. coli cell [3], the Schnakenberg model with spatially inhomogeneous initial conditions [4], and reaction-diffusion systems with reactive boundary conditions [5]. Discussions about the theoretical estimates for the diffusion coefficient based on microscopic dynamics, and methods to simulate a constant diffusion using bath particles will take place.

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# Numerical simulation of mixed convection stagnation-point boundary layer flow and heat transfer of hybrid nanofluids over a vertical plate

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This paper studies the mixed convection flow and heat transfer of  $Al_2O_3$ -Cu/water hybrid nanofluid over a vertical flat plate. Governing equations for conservation of mass, momentum and energy for the hybrid nanofluid over a vertical flat plate are introduced. In order to transform the set of partial differential equations into ordinary differential equations, appropriate similarity transformations are used. Finite-deference with collocation method is used to integrate the governing equations for the velocity and temperature profiles. The results show that dual solution exists for both cases: of assisting flow and opposing flow over the plate.

The governing equations of the conservations of the nanofluids mass, momentum and energy by employing the usual boundary layer approximation are written as:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = g \beta_{hnf} (T - T_{\infty}) + U_e \frac{d U_e}{d x} + \frac{\mu_{hnf}}{\rho_{hnf}} \frac{\partial^2 u}{\partial y^2}$$

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{k_{hnf}}{(\rho C_p)_{hnf}} \frac{\partial^2 T}{\partial y^2}$$

subject to

 $\begin{array}{ll} u=0, \ v=0, \ T=T_w \ (x)=T_\infty + \ T_0 \ (x/L) \\ u\to U_e(x), \ T\to T_\infty & \text{as} \quad y\to\infty \end{array}$ 

A linear stability analysis was performed to identify the stable solution. The results are reported for various volume fraction of composite nanoparticles and mixed convection parameter. The outcomes show that the composition of nanoparticles can notably influence the boundary layer flow and heat transfer profiles. It is also found that trend of the variation of surface skin friction and heat transfer for each of the dual solution branches can be different. The critical values of the mixed convection parameter,  $\lambda$ , where the dual solution branches joint together, is also under the influence of the composition of hybrid nanoparticles. For instance, assuming a total volume fraction of 5% for the mixture of Al<sub>2</sub>O<sub>3</sub> and Cu nanoparticle, the critical value of mixed parameter of  $\lambda$  changes from -3.1940 to -3.2561 by changing the composition of nanofluid from Al<sub>2</sub>O<sub>3</sub> (5%) + Cu (0%) to Al<sub>2</sub>O<sub>3</sub> (2.5%) + Cu (2.5%).

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# The Algorithm Solution of the Problem of Optimal Control in a Dynamic One-Sector Economic Model with a Discrete Time Based on Dynamic Programming Method

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In this paper we study a new formulation of the optimal control problem in a dynamic single-sector economic model with discrete time. In the task, the states are the values of the specific capital, that is, the total amount of capital related to the unit of labor resources. The role of management is played by a parameter representing the proportion of the specific product produced that is directed to investment. The target functionality is the sum of two components. The first one expresses the specific consumption accumulated during the evolution of the system. The second is expressed as a given function of the value of the specific capital at the final point in time and describes the level of technological development in the system formed at that moment. The main limitation is the dynamic ratio for the specific capital, describing its change under the influence of management. The Bellman equations for the problem are obtained. Based on the well-known theoretical assertions, it is established that the sequence of controls satisfying the Bellman equations is optimal. An algorithm has been created and described in detail that allows one to solve the Bellman functional equations numerically and find a sequence of optimal controls for the problem posed.

### From fairness and decisions to a new game theoretic approach

#### D. G. Saari

University of California, Irvine

It is common to model group decisions and interactions among individuals with game theory. Unfortunately, a typical way to understand a game is with an ad hoc analysis, and that can be difficult. In this talk a new "coordinate system" for the space of games (jointly developed with D. Jessie) is introduced, which significantly simplifies the analysis of all games. The reason (as true with any coordinate system) is that the system defines a common systematic (rather than ad hoc) analysis: just express a game of interest in terms of these new coordinates.

Certain coordinate directions, for instance, extract all of a game's information needed to analyze the Nash structure; doing so sharply simplifies computing pure and mixed Nash equilibria. Other directions (orthogonal to Nash information) capture all of a game's traits that involve interactions among the agents, such as coordination, cooperation, and externalities. In an easily computed manner, the coordinates quickly and explicitly display the source of a game's complexities; e.g., coordinates for games such as 'Hawk-Dove, Prisoner's Dilemma, Battle of the Sexes, Stag Hunt immediately exhibit a tension between what individuals can individually achieve (Nash directions) and what a group can attain. Other consequences coming from these new tools are explanations why several measures of complexities and other traits cannot work in general, and ways to analyze games on networks with various topologies.

We look forward to welcoming you in Waterloo, Canada at the AMMCS Conference!

Figure 1: The AMMCS Conference is organized in cooperation with SIAM and AIMS.

# From Celestial Mechanics to the Dark Matter Mystery

D. G. Saari

University of California, Irvine

Following the spirit of Florin Diacu, who would use mathematics to better understand the universe, this talk will use standard mathematical tools of celestial mechanics to address the compelling mystery of dark matter. A strong circumstantial argument used to support the search for dark matter is that if it does not exist, then galaxies must dissipate. As described in this talk, this assertion is *not consistent* with the mathematics of the Newton n-body problem.

We look forward to welcoming you in Waterloo, Canada at the AMMCS Conference!

Figure 1: The AMMCS Conference is organized in cooperation with SIAM and AIMS.

#### Numerical investigation of evaporation of multicomponent droplet

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The main aim of this paper is the numerical investigation of vaporization of a single-component and multi-components fuel droplet as well as a comparison between the effects on the evaporation rates based on the chosen component, that are from different hydrocarbons with low and high volatile (heavier and lighter component). This study considers temperature gradient, species diffusion inside a droplet. Also, the internal recirculation of moving droplet has been taken in to account. While in the majority researches that have been done regarding evaporation of a multicomponent droplet [1,2], transport equations are solved analytically. In this study those equations (1,2) are solved numerically with Finite difference methods.

$$\frac{\partial T}{\partial t} = \alpha \left( \frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) + P(r, t)$$
(1)

$$\frac{\partial Y_{li}}{\partial t} = D_l \left( \frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right)$$
(2)

With respect to the vaporization of droplet, as the radius of droplet is decreasing, it, so the equations (1,2) should be solved with this consideration of moving boundary problem. The dimensionless form of energy equation is derived and then solved. As a result, the boundary condition at surface of the droplet is always added to the same dimensionless parameter. Since the other equation, mass diffusion inside the droplet, the mass fraction is already a dimensionless parameter, it does not need any changes. In this study, evaporation rates of each component are solved individually and validated by experimental data. The effect of different initial portion of each component are discussed. The results show that, adding heavier species with lower volatile to a droplet which contains lighter species can increase evaporation time about 20%, that is illustrated in Figure 1.

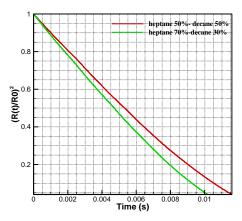


Figure 1-the effect of heaver component with low volatile on evaporation rate.

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# HOW to WRITE DOWN the UNCERTAINTY of MEASUREMENTS, If the FIRST SIGNIFICANT FIGURE is the UNITY

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For all experimentally measured quantities there will always be uncertainties. Estimating the uncertainty is crucial to understanding the measured quantity. In many Physics Laboratory Manuals and Elementary Statistics Guide books the following rules of quoting an experimental uncertainty are recommended. If the first significant figure is the unity, then in the uncertainty two significant figures must be retained. If the first significant figure is not the unity, then in the uncertainty only one [1] or two significant figures must be retained [2].

As a rule, Physics Laboratory Manuals recommend to make from three to five measurements of a quantity. In [3] the formula for estimation the uncertainty in a sample variance was presented, but for correct writing down the measured quantity, it is necessary to know the sample mean value, the standard deviation of the sample mean value and its uncertainty.

In this work, it is shown that the number of significant figures in the uncertainty of the measured quantity is defined by the relative uncertainty in the sample standard deviation of the mean, caused by the finite sample of the size n

$$\delta_{s_{x}^{-}} = \frac{\sigma_{s_{x}^{-}}}{s_{x}^{-}} = \sqrt{\frac{1}{2(n-1)}} \tag{1}$$

For three measurements the relative variance is 50 %, and it does not give the right to retain two significant figures in the uncertainty, even if the first significant figure is unity.

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# **Sparse Estimation for Functional Semiparametric Additive Models**

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We propose a functional semiparametric additive model for the effects of a functional covariate and several scalar covariates and a scalar response. The effect of the functional covariate is modelled nonparametrically, while a linear form is adopted to model the effects of the scalar covariates. This strategy can enhance flexibility in modelling the effect of the functional covariate and maintain interpretability for the effects of scalar covariates simultaneously. We develop the method for estimating the functional semiparametric additive model by smoothing and selecting non-vanishing components for the functional covariate. Asymptotic properties of our method are also established. Two simulation studies are implemented to compare our method with various conventional methods. We demonstrate our method with two real applications.

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# Adiabatic approximation in open quantum systems: applications in quantum computation and quantum thermodynamics

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We provide recent theoretical results and experimental realizations of the adiabatic dynamics in a decohering scenario. We start by considering a formulation for the adiabatic approximation in open quantum systems, which is derived by requiring the decoupling of Jordan blocks of the underlying Liouville superoperator governing the quantum dynamics [1]. Then, we consider the sensitiveness of the adiabatic approximation to resonance conditions [1,2], showing that decoherence may drive the resonant system with high fidelities to the expected adiabatic behavior of open systems. Concerning quantum computation, we consider the adiabatic Deutsch algorithm, where a distinction is established between the open system adiabatic density operator and the target pure state expected in the computation process [1]. As a further analysis, we also present results in quantum thermodynamics [3]. More specifically, we establish heat and work in terms of the underlying Liouville superoperator. As a consequence, we derive the conditions that an adiabatic open system quantum dynamics implies in the absence of heat exchange, providing a connection between quantum and thermal adiabaticity. Experimental realizations for all these applications are then exhibited using a hyperfine energy-level quantum bit of an Ytterbium <sup>171</sup>Yb<sup>+</sup> trapped ion, which provides a highly controllable engineered dynamics.

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#### Variable bandwidth kernels and the UMAP graph construction

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Many authors have studied weighted graph construction methods using variable-bandwidth kernels,

$$W_{\delta}(x,y) = h\left(\frac{d(x,y)^2}{\delta^2 \rho(x)\rho(y)}\right),$$

for some function  $h: [0,\infty) \to [0,\infty)$  with exponential decay, and some local scaling function  $\rho$ . Recently, Berry and Sauer [1] studied the corresponding unweighted graph construction: *x* is connected to *y* if and only if  $d(x,y) < \delta \sqrt{\rho(x)\rho(y)}$ . They show that there is a unique choice of local scaling function  $\rho$  that yields a geometry consistent with the underlying manifold in the limit of large data. This local scaling function is approximated by  $\rho(x) = d(x,x_k)$ , where  $x_k$  is the k-nearest neighbour of *x*. With this choice, the graph construction is called Continuous k-Nearest Neighbours (CkNN).

In a separate development, McInnes et al. [2] have introduced the successful UMAP dimensionality reduction method, which includes a k-neighbour graph construction algorithm corresponding to a kernel function with some similarities to the variable-bandwidth kernels defined above.

We present ongoing work exploring variations of the UMAP and variable-bandwidth kernels, and their corresponding unweighted graph constructions, with numerical applications to topological data analysis and dimensionality reduction.

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#### Convergence of the vanishing physical viscosity limit for gas dynamics

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In this talk, I will describe some recent results, obtained jointly with S. Schulz in [2], concerning the convergence of the vanishing viscosity limit from the compressible Navier-Stokes equations to the compressible Euler equations of gas dynamics in one space dimension. The Euler equations are an archetypal system of conservation laws, used widely in modelling the flow of inviscid fluids. In one dimension and under the assumption of a barotropic flow, the equations take the form

$$\rho_t + (\rho u)_x = 0, \tag{1}$$

$$(\rho u)_t + (\rho u^2 + p(\rho))_x = 0, \tag{2}$$

where  $\rho \ge 0$  is the density of a given fluid, *u* is its velocity, and  $p(\rho)$  is the equation of state determining the pressure. In the case of a viscous flow with viscosity  $\varepsilon$ , an additional term is present in the equation for the velocity, giving the compressible Navier-Stokes equations,

$$\rho_t + (\rho u)_x = 0, \tag{3}$$

$$(\rho u)_t + (\rho u^2 + p(\rho))_x = \varepsilon u_{xx}.$$
(4)

As the Navier-Stokes equations have better regularity properties than those of the underlying Euler equations, they are sometimes used as an approximate system for the purposes of solving the Euler equations. Moreover, it is expected that solutions of the Navier-Stokes equations should converge to solutions of the Euler equations as the viscosity tends to zero, justifying their use as an approximation.

In recent work, jointly with S. Schulz, we have proven the convergence of this vanishing viscosity limit by employing the technique of compensated compactness. In this talk, I will explain some of the main difficulties in treating this limit and how the technique of compensated compactness may be used to overcome these problems in the case of a physically relevant pressure law.

This work is related to a result of Chen and Perepelitsa, [1], for the so-called "gamma-law" gas, in which the pressure is given by  $p(\rho) = \rho^{\gamma}$ . Rather than treat this model case, we consider the physically relevant pressure laws in which the pressure is an approximate gamma-law close to vacuum and grows linearly with the density at high densities. In addition, the results of this work shed significant light on the structure of the entropy functions for the Euler equations with such physical pressure laws.

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# A semi-definite programming formulation for collective mental accounting: an integrated behavioral portfolio selection model

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We present a collective mental accounting (CMA), which integrates all mental sub-portfolios (mental accounts) in one mathematical model. The CMA model can be used to determine the proportions of wealth allocated to each mental account with or without inputs from the investor. Unlike other mental accounting models, it is possible to define constraints on total asset holdings such as short-selling and cardinality constraints in CMA model.

The problem is formulated as a semi-definite programming (SDP) model to make it more tractable and mathematically elegant. We also present a numerical example to investigate the effect of short-selling constraints and compare the portfolio recommendations, utility function, feasibility, and optimality of the CMA with those of existing mental accounting models. The results show that although both types of solutions are meanvariance efficient, CMA results are better in terms of behavioral efficient frontier and utility functions.

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#### A comparison of different trending machine algorithms for energy forecasting

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Accurate prediction of future electricity loads is necessary for the energy industry. Machine learning provides solutions through a variety of algorithms. In this paper we compare the effectiveness of four trending time series ML algorithms - LSTM [1], SVR [2], Xgboost [3], and the Facebook prophet package [4] - for short-term electric load forecasting. We use three different SVR kernels (BFR, linear, polynomial) and investigate their performance.

The models are trained on two years of energy consumption data from the EUNITE competition, and compare the ability of the models to forecast one month of energy consumption. We use the root-mean-square error and mean absolute percentage error metrics to evaluate performance. We find that the best-performing model overall to be the LSTM neural network.

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### A Dynamic Model for Tuberculosis Transmission in Algeria

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Tuberculosis (TB) has emerged as a serious public health problem in Algeria since 1962. The epidemiological surveillance of the disease became operational in 1982 and the data collection became more insightful since 2000. This work aimed at developing a deterministic model for transmission dynamics of TB using the reported data for population and active-TB incidence in Algeria. The stability of equilibria of the built model was investigated and the reproduction number,  $\mathcal{R}$ , was computed. A threshold for the existence of two endemic equilibria for  $\mathcal{R} < 1$  was derived. Sensitivity analyses on the reproduction number with respect to the model parameters were carried out. Some parameters were considered, afterwards, time-dependent. The least-squares fitting have been used for estimating model parameters to the observed data of active-TB incidence in Algeria. Our model agrees well with the observed data.

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# **Quantum Algorithms for a Min-Max Optimization Problem**

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We introduce and analyze two quantum algorithms for solving the min-max optimization problem

$$w_* = \arg\min_{w \in \mathscr{W}} r(w) + \frac{1}{n} \sum_{i=1}^n \max_{y \in \mathscr{Y}} f_i(y, w), \tag{1}$$

where *r* and  $f_i$  are convex functions with Lipschitz continuous gradients, *r* is  $\mu$ -strongly convex,  $\mathscr{Y}$  is a finite set, and  $\mathscr{W} \subseteq \mathbb{R}^D$  is convex. In practice, the size of  $\mathscr{Y}$  could be very large (e.g., exponentially large in terms of the set of rules or the *structure* that describes them) and the dependence of  $f_i(y, w)$  on *y* could be complicated, causing the evaluation of the max operator to be computationally hard. These problems arise frequently in machine learning, for example, in maximum-margin based methods such as SVMs and SSVMs. In these applications  $\mathscr{Y}$  represents a label space, and *w* is a set of tunable parameters (e.g., parameters of a neural network or a probabilistic graphical model). Our two quantum algorithms attain a quadratic speedup over classical algorithms in terms of the size  $|\mathscr{Y}|$ .

Our first algorithm, Q-SubSGDP, based on subgradient descent with polynomial-decay averaging [1], uses the quantum minimum finding algorithm [2] to evaluate the max operator of (1). Our second algorithm, Q-SAGA, is based on the SAGA algorithm [4]. We approximate the non-smooth max operator of (1) with the smooth softmax function, then use the quantum Gibbs sampler of [3] to approximate the softmax function.

**Theorem 1** Given  $\varepsilon > 0$ , *Q*-SubSGDP finds a point  $w \in \mathcal{W}$  satisfying  $|f(w) - f(w_*)| \le \varepsilon$  with high probability using  $\tilde{O}\left(\frac{M|\mathscr{Y}|^{0.5}}{\mu\varepsilon}\log\frac{1}{G}\right)$  queries to the oracles of  $f_i$  with the number of other quantum gates being almost of the same order. G is the minimum gap attained by the functions  $f_i$  for different values of  $y \in \mathscr{Y}$  throughout the runtime, and M is a bound on the  $L^2$  norm of  $\nabla_w[r(w) + f_i(y,w)]$  for all  $y \in \mathscr{Y}$ .

**Theorem 2** Given  $\varepsilon > 0$ , *Q*-SAGA finds a point  $w \in \mathcal{W}$  satisfying  $|f(w) - f(w_*)| \le \varepsilon$  with high probability using

$$\tilde{O}\left(\frac{D^{4.5}\Delta^5|\mathscr{Y}|^{0.5}}{\mu^3\varepsilon^{2.5}}\log n\right)$$

queries to the oracles of  $f_i$  with the number of other quantum gates being almost of the same order, where  $\Delta$  is a bound on the absolute value of the partial derivatives of  $r(w) + f_i(y,w)$  satisfying  $\Delta^2 \leq M \leq D\Delta^2$ .

Both theorems follow from a rigorous analysis of the effect of the errors introduced by the randomized nature of the quantum algorithms used. The quantum minimum finding algorithm used in Theorem 1 can fail to give a correct minimum with a non-zero probability, and the quantum Gibbs sampling algorithm used in Theorem 2 approximates the gradients with respect to w up to an additive error.

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# Multiscale Stochastic Modelling of Cortical Spreading Depression Dynamics in Brain

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Brain activity derives from an interplay of intrinsic dynamics along with stochastic fluctuations. The dynamic processes arise from neurophysiology and anatomical connectivity, while stochastic inputs arise through sensory fluctuations, brainstem discharges and random microscopic states such as thermal noise. The stochastic dynamic models open new opportunities to study the dynamic evolution of systems composed of both random and dynamic fluctuations arising from brain activity [1]. Cortical spreading depression, which occurs in many brain structures, is a slowly propagating wave that causes a drastic failure of the brain hemostasis leading to temporary impairment in the normal functioning of neurons [2]. The clinical disorders related to cortical spreading depression can also lead to pathophysiology of various diseases including migraine, ischemic stroke, transient global amnesia, epilepsy and traumatic brain injury [3]. Importantly, cortical spreading depression is a wave of electrophysiological hyperactivity, whereby neurons are first highly excited that is being followed by a silent phase of membrane hyperpolarization, and later the triggered neurons are slowly recovered to their normal frequencies [3, 4]. The above mentioned neurophysiological phenomenon of cortical spreading depression results in abrupt changes in the intracellular ion gradients, i.e. an increase in extracellular K+ and glutamate, along with rising in intracellular Na+ and Ca2+, followed by sustained depolarization of neurons [2, 3].

In the present study, a more realistic stochastic model of cortical spreading depression propagation in the brain has been developed, considering the synaptic mechanism. The developed model consists of six coupled equations of the reaction-diffusion type in the two-dimensional space and three-parameter Poisson process sources of potassium ions representing extrusions due to the random firing of neurons. Although the overall basic characteristics of cortical spreading depression can be produced by considering only potassium and calcium ion concentrations, we have considered a more comprehensive model of 4 ions: K+, Na+, Ca2+, Cl+, excitatory transmitter representing glutamate and inhibitory transmitter representing gamma-Aminobutyric acid. The developed model is expected to reproduce many important characteristics of cortical spreading depression of cortical spreading depression has also been evaluated. Lastly, a comparative study has been conducted to highlight the significance of a stochastic modeling approach to cortical spreading depression propagation versus deterministic approaches. It is expected that the developed model will provide a more comprehensive understanding of the key mechanisms underlying the dynamics of the pathological brain.

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# Differential capacitance of ionic liquid interface with graphene: the effects of correlation and finite size of ions

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Graphene has shown great potential for applications in biological and chemical sensing due to its unique electronic band structure [1, 2]. Graphene based sensors typically operate as Field Effective Transistors with the graphene layer operating as the conducting channel with an electrolyte solution as its gate [3]. Recently, there has been a peak in interest in studying the electric double layer that arises at the interface of doped graphene and a class of electrolytes known as ionic liquids. Ionic liquids are a class of ionic salts that are molten at room temperature with low volatility and high ionic concentration[4, 5], and are characterized by the overscreening and overcrowding effects in their electric double layer [6].

In this work, a mean field model for ionic liquids is presented. This model takes into account both the ion correlation and the finite ion size effects. A computational procedure has been developed in order to calculate the differential capacitance of the ionic liquid interface with single-layer graphene. The role of the ion packing on the transition from Camel to Bell shapes in the diffuse layer is analyzed. Next, the effect of the ion packing fraction and the correlation lengths on the fraction of the potential that goes into charging the graphene electrode is analyzed. In addition, we explore small packing fractions in the dilute electrolyte regime and we extended those results for asymmetric ionic liquids. We show that the main effect of a graphene electrode versus a metallic one arises due to a V-shaped minimum in its quantum capacitance due to the Dirac cone structure of graphene's  $\pi$  electron bands. Consequently, the total interfacial capacitance exhibits a Camel-shaped dependence on the potential applied to the system, even for large ion packing fractions and finite correlation lengths.

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# Differential equation model for the treatment of tumor growth with the effect of immune response with radiotherapy

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Radiation therapy is a certain type of energy to kill cancer cells and shrink tumors; it destroys cells in the area being treated by damaging their genetic material. The radiation damages both kinds of cells, cancer cells and normal cells. Hence nowadays there is rapidly growing interest in the potential for synergistic, clinically relevant therapeutic responses by combining radiation therapy with immune response. A new mathematical model of radio-immunotherapy for tumor treatment was introduced. In this work, the linear and exponential spatial dependence of tumor parameters was used. The dose distributions model of radiotherapy with immune response for tumor treatment was formulated. A discussion, on the effect of immune response with radiotherapy for the treatment of tumor is explained in details.

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# Mathematical Modeling of Integrated Pest Management with Stage Structuring and Impulsive Control

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People from different eras associated with agriculture used their own technology and methodology to control the pests. With the passage of time and development of agriculture, science and technology, a number of pesticides have been formulated which can kill the pests rapidly and are exhaustively used by farmers. But from last few decades, it has been observed that the pollution caused by pesticides is dangerous and has desperately damaged the health of human beings and of other creatures of the world. Moreover, recent study shows that with regular use of pesticides, a number of pests have become resistant to some pesticides. This leads to farmers' loss and forces them to use strong pesticides. The aim of this paper is to study a stage-structured integrated pest management model(biological and chemical) to control agriculture pests effectively, economically and safely. Stage structuring is proposed due to the fact that almost all the pests in their life pass through two stages namely, immature larva and mature adult. we purpose a pest control model with stage structuring in pests and natural enemies in the presence of impulsively released natural enemy and chemical pesticides. All positive solutions are proved to be uniformly ultimately bounded. The stability analysis of pest extinction periodic solution, as well as the permanence of system, are obtained by making use of floquet's theory, small amplitude perturbation technique, and comparison theorem. The results obtained provide certain dependable theoretical findings for effective pest management. At last, theoretical findings are confirmed by means of numerical simulation (see Fig. 1).

Key words: Pest Management, Stage Structure, Impulsive Differential Equations, Stability.

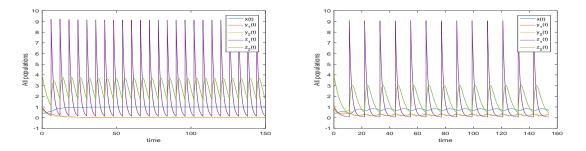


Figure 1: Stability of pest extinction periodic solution and permanence of system.

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# Global Riemann solver for 3x3 system of conservation laws with degeneracy

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A main building block for the analysis of hyperbolic conservation laws is the solution of the Riemann problem, where the initial data are piecewise constant. In general, when the flux is nonlinear and the system is hyperbolic, solutions for Riemann problems only exist for small initial data. In this talk we consider several 3x3 systems of conservation, some from reservoir simulation and some from traffic flow, where the eigenvalues of different family change their ordering. Such systems are parabolic degenerate. Thanks to special features in the models, such as a decoupling property in a certain Lagrangian coordinate, we construct global Riemann solvers. Further research topics for these equations will also be discussed.

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#### Optimal control of quantum spin chains

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Control of quantum systems, both in theory and applications, attracts considerable attention of researchers. The abilities of producing and transforming desired quantum states become critically important for the development of quantum information technologies. The studies in this field are usually related to evolution of various systems under time-dependent Hamiltonians and preparation of the desired final states of this evolution with the highest possible fidelity. These transformations have to be performed sufficiently fast to overcome detrimental effects of decoherence on longer time scales. Therefore, slow adiabatic processes, theoretically providing a high fidelity, are not good candidates for the system evolution.

Here we present analysis of evolution of quantum spin 1/2 systems, considered as promising hardware elements for quantum computing, both in the antiferromagnetic quantum Ising and Heisenberg coupling realizations in external magnetic fields. The operations we consider are local "cutting" and "stitching", that is decrease of the spin-spin exchange coupling from its initial value *J* to zero and from zero to *J*, respectively. This first controlled set of operations is cutting of a bond separating a single spin from a linear chain, or of two neighboring bonds for a ring-shaped array of spins. We show that the disconnected spin can be in the ground state with a high fidelity even after a non-adiabatic process. Next, we consider inverse operation of stitching these bonds to increase the number of connected spins in the system. Another set of examples is transformations from a closed ring-like to an open spin chain and *vice versa* produced by modification of a single link strength in a pair of neighboring spins.

We show that the optimal control algorithm can in general be found by using common numerical procedures with a simple multi-parametric control (with two or three free parameters) function g(t) able to produce high (> 0.99)-fidelity local operations. Therefore, the fidelity of such a transformation can be increased in the nonadiabatic time domain by proper choosing of g(t)J for the time-dependent spin-spin exchange coupling. We obtained numerically this function for two realizations of spin chains (up to 10 spins included) and all the sets of local transformations of interest. On this basis, we present heuristic reasons restricting possible time-dependence of the Hamiltonians applied for achieving a high-fidelity spin chain manipulation.

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#### Reducibility of the Fermi surface for periodic graph operators

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For a periodic Schrödinger or elliptic operator, the Fermi surface for a given energy E is the analytic set in  $\mathbb{C}^2$  of all wave vectors admissible by the operator at that energy. This investigation develops and applies analytical techniques to determine the reducibility of the Fermi surface and to construct periodic graph operators whose Fermi surface is reducible at all energies.

The reducibility of the Fermi surface is fundamental to the study of embedded eigenvalues of locally perturbed periodic operators. It is therefore important for the study of resonant scattering of waves in periodic media when the underlying operator is a perturbation of one that admits an embedded eigenvalue. Specifically, it is known that it necessary that the Fermi surface be reducible at a given energy E in order for a local defect to engender an embedded eigenvalue at E with square integrable eigenfunction having unbounded support [2].

Although non-generic, the reducibility of the Fermi surface is a commoner phenomenon than the decomposition of a periodic operator into simpler periodic operators. We address three aspects of the reducibility of the Fermi surface for discrete and metric graph operators.

(1) By coupling two copies of a metric graph with identical periodic Schrödinger operator by attaching edges between corresponding vertices, the Fermi surface becomes reducible at all energies whenever a certain spectral asymmetry function is identical for all the coupling potentials on the connecting edges [4].

(2) We develop a computational algorithm for computing the Fermi surface of Schrödinger operators on metric graphs in terms of the Fermi surfaces of subgraphs. By this method, the Fermi surface of multi-layer AA- or AB-stacked graphene is shown to have several components [1].

(3) The Fermi surface of a connected doubly periodic self-adjoint discrete graph operator is irreducible at all energies provided that the graph (a) can be drawn in the plane without crossing edges, (b) has positive coupling coefficients, (c) has two vertices per period. This is proved by reduction to sixteen isomorphism classes and the use of Groebner bases [3].

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### **Towards High-Order Meshes of the Cardiac Anatomy**

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Accurate physiological simulations require highly-accurate geometric models of the patient anatomy and implanted medical devices (as appropriate). High-order finite element methods can be used to perform the physiological simulations. Such methods obtain additional accuracy by increasing the polynomial degree of the basis function associated with each mesh element. This requires a corresponding elevation of the polynomial degree of the meshes used to represent the geometric models. High-order meshes can then be used to represent a curved geometry with many fewer elements and hence result in a computational savings when coupled with high-order finite element methods.

We are interested in performing computer simulations in order to quantify the active stresses in the heart from the tissue displacement data acquired using medical imaging in order to assess direct, cardiac biomechanical function. This assessment of cardiac biomechanical function can be used to predict which portions of a heart are damaged/diseased. Such simulations require dynamic, high-quality, high-order curvilinear meshes of the cardiac anatomy throughout the heartbeat cycle.

In this talk, we will describe our approach for generating high-order curvilinear meshes of the myocardium. Our triangular/tetrahedral advancing front method is a direct mesh generation approach which aims to generate high-quality mesh elements at the time of generation so that post-processing is not required. This is in contrast with other high-order mesh generation algorithms which typically deform an enriched linear mesh of the geometry into a high-order, curvilinear mesh. Such methods often require mesh untangling as a post-processing step.

As time permits, we will also summarize our earlier, *a priori* approaches for generation of high-order curvilinear meshes as applied to the myocardium. These optimization-based approaches generate high-order triangular/tetrahedral, curvilinear meshes by deforming an enriched linear mesh into a high-order mesh. The methods employ either an affine [1] or a convex [2] combination of the nodal positions of the interior nodes' neighbors in order to move the interior nodes to new locations. Both methods require mesh untangling as a post-processing step.

We will conclude by identifying several possibilities for future work in the area of generation of high-order curvilinear meshes for cardiac anatomies.

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### Models of Swimming Bacteria with Two Flagellar Bundles

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Microrobots currently hold great interest within the academic community for their potential in biomedical and other fields [1]. For example, microrobots could be used for targetted drug delivery and performing minimally invasive surgery. An important aspect of functionality for such microrobots is motility. We focus on a class of propulsion mechanisms inspired by motile bacteria, namely, flagellar propulsion. Bacterial swimming has been extensively studied in experiments and simulations, yet, the wide range of variations in motility patterns observed across species is not well understood.

We adapt a classic model for propulsion of a spheroidal cell body by a turning, corkscrew-shaped flagellum [2]. The velocities of the organism are obtained by numerically solving the equations of fluid flow in the Stokesian regime with no-slip boundary conditions imposed on the surface of the cell body and flagellum. A boundary element method is used for accurate numerical solutions and comparisons are also made with fast schemes based on resistive force theory and multipole expansions.

In this study, we investigate the consequences of adding a second flagellum to the bacterial cell [3]. This is motivated by strains of magnetotactic bacteria that swim with two flagellar bundles [4]. Analyzing the simulated motion in bulk fluid and close to solid surfaces, we show that the placement of the two flagella on the organism affects both the rate of rotation of the body and the swimming speed. Near surfaces, the flagellar configuration has an even more dramatic effect, determining the direction and magnitude of curved trajectories parallel to the plane of the wall, as well as motion away or towards the wall. Evidently, swimming with two flagellar bundles rather than one confers more potential benefits than simply greater thrust. This is of significance not only for understanding differences in bacterial morphology but also for designing microrobots that can swim controllably in confined environments.

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# Mathematical Modeling of Electro-thermal Response on Nerve Tissue Subjected to Radiofrequency Field

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The application of radiofrequency electric signals to neural tissues is one of the most common and auspicious methods used to treat pain, movement and disorders. The radiofrequency power deposited within the tissue during such therapy provokes the temperature rise above the lethal temperature range (i.e. at or above 45-50 °C) near radiofrequency electrodes, destroying the adjacent cellular structures [1, 2]. Moreover, the rise in tissue temperature during such thermal therapy could also lead to induction of nociceptive pain. Importantly, the transduction of nociceptive pain occurs through the nociceptors that reside on the ends of the long axons of neurons. The function of nociceptors depends on the ion channels that mediate the selective passage of specific ions or molecules across cell membranes at noxious temperature levels. The nociceptors are one of the three kinds of peripheral nerves: myelinated afferent  $A\delta$  and  $A\alpha$  fibers; and unmyelinated C afferent fibers, and the thermal pain sensations are mainly mediated by both myelinated  $A\delta$  and unmyelinated C fibers [3, 4].

In the present study, a mathematical model has been developed to take into account the effects of thermal pain sensation induced during the radiofrequency heating of the neural tissue. A three-dimensional computational model comprising of neuromuscular tissue has been considered in which the radiofrequency electrodes have been inserted. A finite-element-based implementation has been used to solve the proposed electrothermo-neural model. Importantly, the main governing equations of the multi-scale and multi-physics model are: (a) a simplified version of Maxwell's equation utilizing quasi-static approximation for estimating the electric field distribution, (b) Pennes bioheat transfer equation for estimating the temperature distribution and (c) modified Hodgkin-Huxley model for prediction of nociceptor electrophysiology from the ionic currents. The temperature-controlled radiofrequency has been modelled on the neural tissue utilizing the clinical protocols applied in actual practices along with taking into account the temperature-dependent electrical and thermal conductivities. The effects of different sizes of nerve fibers and different values of target tip temperature have also been quantified. It has been found that the postoperative thermal pain is significantly dependent on the duration and magnitude of target tip temperature during the radiofrequency heating of nerve tissues. These new findings and associated quantifications based on our numerical studies will provide a much better understanding of nociceptor signaling subjected to high temperatures during such therapies. Moreover, the advancement and extension of the developed mathematical model can assist further in analyzing, predicting and mitigating chronic pain, its management and ultimate control.

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# **Experimental Detection of Qubit-Ququart Pseudo-Bound Entanglement using Three Nuclear Spins**

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In this work, we experimentally created and characterized a class of qubit-ququart PPT (positive under partial transpose) entangled states using three nuclear spins on an nuclear magnetic resonance (NMR) quantum information processor [1]. Entanglement detection and characterization for systems with a Hilbert space dimension > 2  $\otimes$  3 is nontrivial since there are states in such systems which are both PPT as well as entangled. The experimental detection scheme that we devised for the detection of qubit-ququart PPT entanglement was based on the measurement of three Pauli operators with high precision, and is a key ingredient of the protocol in detecting entanglement [2]. The family of PPT-entangled states considered in the current study are incoherent mixtures of five pure states. All the five states were prepared with high fidelities and the resulting PPT entangled states were prepared with mean fidelity  $\geq$  0.95. The entanglement thus detected was validated by carrying out full quantum state tomography (QST).

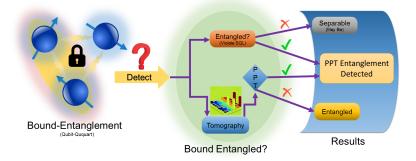


Figure 1: Schematic of the Pseudo-Bound-Entanglement detection procedure.

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# The dynamics of the quantum correlations measured by the local quantum uncertainty and trace distance discord for the bipartite X states

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**Abstract**: Recently, quantum correlations have been the subject of deep studies, principally due to the general belief that they are fundamental resources for different quantum, information processing tasks. These correlations are difficult to maintain because a quantum system is usually not closed, but in interaction with its environment. In this in work, we employ the concept of local quantum uncertainty (LQU) and trace quantum discord (TQD) to investigate the environmental effects on quantum correlations of a two qubit system. Two decoherence scenarios are considered. The first one concerns the coupling of the system with two independent bosonic reservoirs. The second scenario deals with a two level system interacting with a quantized electromagnetic radiation.

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Peristaltic Transport of an Ellis Fluid in an Inclined Asymmetric Channel

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Peristaltic transport of an incompressible Ellis fluid, in an inclined asymmetric channel is studied under low Reynolds number and long wavelength assumptions. The walls were assumed as an infinite train of sinusoidal waves, both traveling at a constant speed and having the same wavelength. Expressions for the axial and transverse velocities, volume flow rate, pressure rise per unit wavelength and streamlines are obtained. The effects of the wave amplitudes, the phase difference, the channel width, the angle of inclination of the channel and the fluid parameters on the flow were observed. The conditions necessary for trapping to occur were also explored. It was observed that changes in the fluid conditions that deviated from the Newtonian condition resulted in a decrease in the axial velocity closer to the center of the channel and a simultaneous increase in the velocity closer to the walls of the channel. The pressure rise per unit wavelength has a non-linear relation with the volume flow rate, which became more pronounced with an increase in the absolute value of the volume flow rate. The Newtonian case however, displayed a linear relation between the two variables. The streamlines and hence the trapped region are affected significantly by the wave amplitudes, volume flow, channel width and phase difference of the waves and less by the fluid parameters.

# A Hamiltonian framework for the problems of economic growth theory

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We introduce a general Hamiltonian framework that appears to be a natural setting for the derivation of various production functions in economic growth theory, starting with the celebrated Cobb-Douglas function. Employing our method, we investigate some existing models and propose a new one as special cases of the general *n*-dimensional Lotka-Volterra system of eco-dynamics.

Joint work with Kunpeng Wang

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# In search of a new economic model determined by logistic growth

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We propose a new growth model based on the assumption of logistic growth in factors. The model is an extension of the work by Sato devoted to the development of economic growth models within the framework of the Lie group theory. It is employed to derive new production functions and introduce a new notion of wage share.

We will discuss one of these production functions in relation to the "S-shaped" production function that has been recently introduced within a similar context and extensively studied in works by Anita, Capasso, Engbers, Kunze, La Torre and others.

We will also show that the new functions compare reasonably well against relevant economic data. In addition, we will explain in reasonably rigorous mathematical terms why Bowleyâs law no longer holds true in post-1960 data.

Joint work with Kunpeng Wang

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# Long-time asymptotics for some nonlinear wave equations with variable propagation speeds

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This talk is concerned with wave equations in one space dimension of the form

$$\partial_t^2 \phi - c^2(x) \partial_t^2 \phi = N(\phi),$$

where the propagation speed c(x) is a small perturbation of the constant  $c \equiv 1$ .

First, we discuss the case  $N(\phi) = \phi - \phi^3$ , known as the  $\phi^4$  model. When  $c \equiv 1$ , a stationary solution called the *kink* is known explicitly, and this solution has been shown to be asymptotically stable with respect to odd perturbations by Kowalczyk, Martel, and Muñoz [1]. We will discuss the extension of this asymptotic stability result to the case where c(x) is sufficiently close to a constant. A precise understanding of the spectrum of the linearization around the variable-speed kink is an important element of this analysis. These results were published in [2].

Next, we will discuss ongoing work (joint with M. Alammari) on the case  $N(\phi) = -\sin(\phi)$ , the sine-Gordon equation. Although this equation has some features in common with the  $\phi^4$  model, the constant-speed kink is in fact not asymptotically stable because of the presence of breathers. It is not *a priori* obvious whether this property will be preserved under any small perturbations of the propagation speed. We will explain how adapting and extending the methods of [2] to study the linearization around the kink can shed light on this question.

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# Thermodynamic Simulation of Heavy Oil Upgrading

in Supercritical Water Using Aspen Software

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The energy crisis and environment pollution are two serious problems that are of great concern all around the world. Thus seeking for development of novel and green chemical processes gain rising attention. Here, water at elevated pressures and temperatures above the critical point (374°C, 22.1MPa), namely supercritical water (SCW), is highly promising and efficient for carrying out chemical reactions. The physicochemical proprties of water like polarity, density, solubility, viscosity, surface tension and ionization, change dramatically which adapt it as a nice candidate for processing of petroleum heavy oil (HO) utilizing both physical (solvation) and chemical (as hydrogen donor) properties of SCW. The present study considers the thermodynamic simulation of heavy oil upgrading in SCW in the presence of oxygen using Aspen software. Set of experiments was conducted in order to compare the simulation and experimental results as well. The aim was seeking the upgrading condition where light hydrocarbons form CO by the help of partial oxidation and later created in-situ active hydrogen from water gas shift reaction  $(CO+H_2O\rightarrow H_2+CO_2)$  for effective hydrogenation of heavy oil in SCW with less coke. Applying powerful capability of Aspen plus, i.e., sensitivity analysis, the effect of significant parameters, such as temperature, pressure (water density), water to oil ratio, and  $O_2$  to oil ratio were studied comprehensively in order to maximize the amount of active hydrogen. The results indicate that higher temperature as well as the amount of water are favorable for increasing the contribution of active hydrogen, while the pressure is not determining factor at supercritical condition (P>25MPa). The formation of methane was also decreased at high temperature which is desired for upgrading system. The higher amount of water implies more quantity of  $O_2$  since partial oxidation affords the enthalpy of auto-thermal reforming of HO. Hence there should be a compromise in the selected ratios of H<sub>2</sub>O/HO and O<sub>2</sub>/HO in SCW upgrading system. Although the experiment results are established on kinetic data which also reflect the physical effect of SCW during upgrading, however, the thermodynamic study were achieved by Aspen simulation, provides valued information, in agreement with experiments, that improves our understanding of heavy oil upgrading in SCW.

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#### On the modeling of drug delivery to solid tumors; computational viewpoint

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Drug distribution in a solid tumor is important in evaluation of the cancer treatment efficacy. In the present study, a comprehensive fully-developed multi-scale mathematical model including Darcy's law, Starling's approximation, and Fick's law are respectively employed to calculate the interstitial fluid pressure (IFP) and drug distribution in interstitial space. The computational approach considered the mechanisms of convection and diffusion of drug in interstitium and drug extravasation from microvessels or to lymphatic vessels. Two different zones including necrotic core and semi-necrotic zone are considered for a tumor which surrounded by normal tissue. The transient distribution of drug concentration is calculated based on the IFV and IFP distribution. The results indicate that drug concentration has its maximum value in the semi-necrotic region and it starts declining steeply in the necrotic region of the tumor. Simulation results also show that there is a critical size for necrotic core radius. Below this size, changing the necrotic core radius had a limited impact on IFP, IFV, and drug distribution, while for the radius above this critical size, the simulated drug distribution is significantly influenced by the size of necrotic core. The outputs of such model provides more insight in the drug delivery and transport to solid tumors during chemotherapy.

Keywords: Drug delivery, Solid tumor, Porous media, Necrotic core, Drug concentration.

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#### Thermodynamic analysis of a commercialized CAES plant and improving Round Trip Efficiency using low grade waste heat as steam generation heat source

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Compressed Air Energy Storage (CAES) is a technique to move demands from peak to off-peak times. This method of energy storage would reduce cost of power generation and facilitate demand responses where renewable types of energy are utilized as the main source. Hence, the precise study of parameters affecting CAES performance and ways to improve its efficiency have been the main goals of researchers in recent years.

At present work, a Thermo-Exergetic study of a conventional CAES with multi-stage compression, four inter/after-stages cooling and two turbines has been implemented to verify the solution procedure. The simulation showed appropriate accordance with actual data presented in [1].

The effect of thermodynamic conditions of compression/expansion train, ambient air sensitivity and exergy analysis versus plant performance has been presented in a set of graphs. For instance, the relative humidity study indicates that after occurrence of wet compression phenomena inside compressors the thermal efficiency and compressor power consumption has remarkably been improved, see Figure 1.

After a concise preamble about common ways of RTE enhancement [2], the influence of exhaust air recovery and addition of water to operative fluid has been studied on plant performance. Water injection study shows that input work has been noticeably reduced, but the outlet power after a small increase remained constant due to condensation and sedimentation of water vapour in caverns. Hence, this mass flow subtraction has been recovered by steam injection in combustion chambers which is generated using low grade waste heat. Also, the effect of regeneration has been investigated. It has been observed that recuperation with approach temperature of 10 °C would increase RTE about 10%. Finally, the combined effect of regeneration and steam/water injection on input/output power and RTE has been investigated and optimized system is proposed.

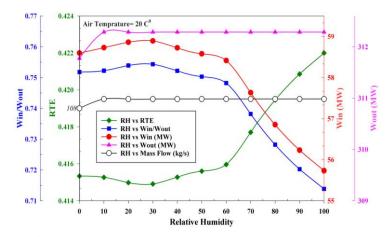


Figure 1: The RH effect on inlet/outlet power, RTE, and power ratio

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# Entangling continuous variables with a qubit array

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We show that an array of qubits embedded in a waveguide can emit entangled pairs of microwave photon beams. The quadratures obtained from a homodyne detection of these outputs beams form a pair of correlated continuous variables similarly to the EPR experiment. The photon pairs are produced by the decay of plasmon-like collective excitations in the qubit array. The maximum intensity of the resulting beams is only bounded by the number of emitters. We calculate the excitation decay rate both into a continuum of photon state and into a one-mode cavity. We also determine the frequency of Rabi-like oscillations resulting from a detuning.

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#### Perturbing Hamiltonians via automorphisms of the torus

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A study of perturbations of Hamiltonians plays an important role in Quantum Theory and in its applications to Condensed Matter Physics, Materials Science, Chemistry, Synchrotron Science, etc. The traditional approach goes back to the 1930s work of E. Wigner, H. A. Jahn, E. Teller, and others, and focuses on the action of symmetry groups, and the concept of symmetry breaking. In this talk I will present an *alternative approach*. It is based on an observation that a Hilbert space operator can be perturbed via torus automorphisms; in particular, via cyclic shifts or via automorphisms identified with elements of GL(2,Z) (the group of 2 by 2 matrices with integral entries and of determinant  $\pm 1$ ).

The general concepts will be illustrated via a particular example of a quantum structure; namely, a continuous variable approximation of a qubit array, developed jointly with A. Zagoskin, [1]. Remarkably, a complete analysis of this essentially solvable model naturally involves wavelets and fractals. As it turns out, perturbations of some nontrivial operators underlying this model also possess rare properties, e.g. see Fig. 1. In particular, a perturbation of an operator with a connected interval spectrum may have a gapped spectrum. (Note that there is no periodic potential involved.)

This is a new research direction which relies upon the concept of Q-transform, [2]. While an in-depth physical interpretation of the Q-transform is not yet fully understood, the proposed perturbation technique may be used already, particularly in investigations of the structure of materials and quantum processes alike. The envisioned method involves switching from the bottom-up to a top-down approach. Namely, in most of the classical science one constructs models starting from the fundamental principles and gradually adding structure. In contrast, modern computational optimization methods enable one to construct models based on the best fit to (whatever type of) data, notwithstanding that the results need not be easy to interpret via the fundamental principles. A combination of these concepts suggests a method for finding the best model among the specific perturbations considered here.

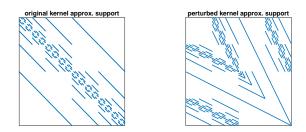


Figure 1: The left graph shows the approximate support in the torus  $[0,1]^{\times 2}$  of the distributional kernel of the original operator. The right graph shows the approximate support of the operator perturbed by the matrix T = [1,1;0,1].

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# Computer science techniques for species classification

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Lake whitefish (*Coregonus clupeaformis*) are a primary support for subsistence and commercial fishing in Canada. In the 20th century, lake whitefish populations experienced a dramatic decline as a result of overfishing, environmental degradation, and predation. With proper environmental management and fishery management, populations have recovered, however certain local populations are still at risk. To properly manage these fisheries for sustainable yield, it is important that the genetic diversity of the populations is maintained to ensure evolutionary potential of the species.

In this talk, we consider novel techniques from mathematics, statistics, and computer science, such as machine learning, that can be used to classify species based on genetic sequences extracted from environmental DNA. We investigate and compare the efficacy of these techniques, based on an array of criteria including data size requirements, method accuracy, method speed, and specific obstacles to the application of each method. Any preliminary results on the application of the methods to classify species will be presented.

# Theory of optimization-constrained differential equations

#### P. Stechlinski<sup>1</sup>

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Foundational theory is given for differential equations constrained by nonlinear optimization problems. Motivated by problems with incomplete information found in systems biology and atmospheric chemistry, this modeling framework exhibits nonsmoothness because of active constraint changes in the embedded optimization problem. This hybrid-like behavior (i.e., a mixture of continuous behavior and discrete events) can cause failure of conventional dynamic simulation and optimization methods. The approach here is to consider the optimality conditions associated with the optimization problem, resulting in a nonsmooth differential-algebraic equation system. Well-posedness and sensitivity analysis theory are established, under mild regularity conditions, which mirror classical theory. This is accomplished using recent results in nonsmooth analysis, including lexicographic differentiation, and nonsmooth dynamical systems. The theory outlined here is computationally relevant as it allows for practically implementable methods to be developed; the sensitivity information furnished from this approach can be supplied to dedicated nonsmooth numerical methods.

# Strategic Voting and Black's Condorcet-or-Borda Voting System

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In 1958, Duncan Black proposed a method for electing one winner from three or more candidates. Each voter ranks all of the candidates. If there is a Condorcet winner, that candidate is elected; otherwise, the winner is determined by Borda count. More recently the system has been championed in lectures and articles by Eric Maskin. Maskin calls the system "true majority rule" and emphasizes the merits of picking a Condorcet winner, arguing that in modern political contests, Condorcet cycles are unlikely.

We test that proposition by analyzing several specific scenarios, taking for granted that voters will form factions and vote strategically when it is practical for them to do so. We regard strategies as practical if they do not rely on unrealistically precise polls, and if they either (a) involve only a few ballots or (b) are simple and public. For example, it is practical for voters to form the habit of listing their candidates' most dangerous rivals last, regardless of actual preference.

We focus on three election scenarios: Two major candidates plus minor "spoiler" candidates; two major candidates and a serious "middle" candidate; and three candidates, two of whom can be seen as splitting the votes of a majority party. All of these cases occur regularly and cause controversies in practice.

In each scenario, we find circumstances in which a faction that prefers its prospects in the Borda count can vote strategically in a way that prevents the emergence of a Condorcet winner. It can happen that a candidate would be a Condorcet winner according to the voters' sincere preferences, but is not assured of winning when the Condorcet and Borda methods are combined in this way.

Of course all systems can produce controversial results. Nothing in these results should discourage us from seeking a Condorcet winner, perhaps with a different backup system in place of the Borda count. But whatever the backup system, we should be aware of the possibility that factions that prefer their chances under the backup system can find strategies to enforce its application.

### Option Pricing under regime-switching jump-diffusion model using CLMR tree

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The classical Black-Scholes formula for option pricing uses a Geometric Brownian Motion model to capture price dynamics of the underlying asset. However, it is well known that the stochastic variability in the market parameters is not reflected in the BS model. In recent years, considerable attention has been drawn to regime-switching models which can solve this problem. Furthermore, the necessity of taking into account large market movements, as well as a great amount of information arriving suddenly(i.e. a jump) has led to add the jump into the regime-switching model. And that is called regime-switching jump diffusion model. And here is the definition of this model:

On a filtered probability space  $(\Omega, \mathscr{F}, \mathscr{P})$ , the asset price follows the following process

$$S(t) = e^{X(t)}.$$

where X(t) is specified as the following regime-switching jump-diffusion model,

$$\begin{cases} dX(t) = [\varepsilon_l - \lambda_l m_l] dt + \sigma_l dW(t) + dJ(t), \\ X(0) = \ln S(0), \end{cases}$$
(1)

where for each regime  $l \in D$ ,  $\varepsilon_l = r_l - \sigma_l^2/2$ ,  $m_l := E[e^{Z_1^l} - 1]$ ,  $\sigma_l$  is the volatility and W(t) is a standard Brownian motion under the pricing measure. Furthermore, J(t) represents the cumulative jumps by time t,  $J(t) = \sum_{k=1}^{N(t)} Z_k^{\alpha(\tau_k)}$ , where  $\tau_k$  denotes the *k*-th jump time of the Poisson process  $N(\cdot)$ .

In this paper, we study the convergence rates of the multinomial trees constructed by [*Costabile, Leccadito, Massabó and Russo, Journal of Computational and Applied Mathematics, 256 (2014), 152 - 167*] for European option pricing under the regime-switching jump-diffusion model, which is named as CLMR tree. We also extend the CLMR tree to the pricing of Asian options under the models. Numerical examples are carried out to confirm the theoretical results and the accuracy of computation.

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### On the Optimal Shape of Tree Roots and Branches

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In this talk, We introduce two classes of variational problems, determining optimal shapes for tree roots and branches. Given a measure  $\mu$ , describing the distribution of leaves, we introduce a sunlight functional  $\mathscr{S}(\mu)$  computing the total amount of light captured by the leaves. On the other hand, given a measure  $\mu$  describing the distribution of root hair cells, we consider a harvest functional  $\mathscr{H}(\mu)$  computing the total amount of water and nutrients gathered by the roots. In both cases, we seek to maximize these functionals subject to a ramified transportation cost, for transporting nutrients from the roots to the trunk and from the trunk to the leaves. The main results establish various properties of these functionals, and the existence of optimal distributions. In particular, we prove the upper semicontinuity of  $\mathscr{S}$  and  $\mathscr{H}$ , together with a priori estimates on the support of optimal distributions.

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# **Endowment Manipulations in Probabilistic Assignment Problem**

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For probabilistic assignment, we investigate the existence of rules which satisfy efficiency, the "endowment lower bound", one of several types of endowment manipulations. There are indeed various ways in which an agent can manipulate his endowment. An agent may manipulate a rule on his own, or in conjunction with others. We study three types of individual endowment manipulations and seven types of coordinated endowment manipulations. We prove a combination of positive and negative results concerning the existence of rules satisfying efficiency, the endowment lower bound, and each one of these manipulations. Each of "exchange-proofness", "withdrawing-proofness", "pre-delivery-proofness", and "merging-proofness" are incompatible with efficiency, the endowment lower bound, and a weak fairness property. We propose two rules, which both satisfy efficiency and the endowment lower bound, and each of them is immune to certain types of endowment manipulations.

# Scale-dependent hyperbolic models and well-controlled dissipation schemes

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We consider nonlinear hyperbolic systems of conservation laws endowed with a convex entropy pair and their weak solutions depending upon small-scale parameters. We design numerical schemes for the approximation of these weak solutions, which may contain nonclassical shock waves driven by diffusive-dispersive effects. We introduce a general class of schemes satisfying a discrete form of the system of diffusive-dispersive conservation laws, a discrete form of the associated entropy inequality, and which are consistent with a given system at arbitrarily high-order accuracy. We investigate several hyperbolic models arising in continuum physics. We perform numerical experiments which demonstrate that the proposed schemes are robust and accurate and allow us to compute entropy solutions containing nonclassical shock waves.

# Model of Quorum Sensing Inhibitors as Adjuvants to Antimicrobials in a Chemostat

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Bacterial cells can coordinate group behaviours through a cell-to-cell communication mechanism known as Quorum Sensing (QS). This method is based on the local density of a cell population. Bacterial cells continuously produce and release signal molecules, called autoinducers (AIs). Once these molecules exceed a certain threshold, down-regulated cells begin to up-regulate and induce a switch in group behaviour. For instance, they might switch from a mode of fast growth to a mode of slow growth where resources are invested into protection mechanisms. In areas where bacterial growth is harmful, it has been suggested that interfering with the QS mechanism might make it easier to control microbial growth. Quorum Sensing Inhibitors (QSIs) have been proposed as adjuvants to antimicrobial therapies. They dock onto cell receptors and prevent the bacteria from responding to AIs. Thus keeping a larger part of the population in a down-regulated, unprotected mode of growth.

We formulate a mathematical model for such quorum sensing for a bacterial population in a chemostat setup. To this end, we subdivide the population into down-regulated cells, up-regulated cells, and cells that are blocked from up-regulation by QSIs. We also track a growth controlling nutrient, the concentration of AIs, QSIs and antimicrobials. We investigate this seven dimensional ODE model with a blend of analytical and numerical techniques.

Our focus is on the role of the operating conditions of the reactor. For example, Figure 1, explores the effects of increasing the flow rate on the size of each cell sub-population. With our model we are able to explore ranges of reactor operating conditions in which quorum sensing inhibition strategies are promising.

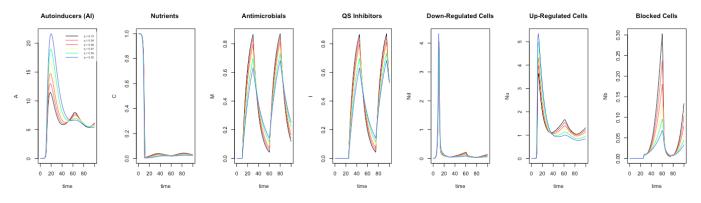


Figure 1: Changes to the ODE model when increasing the flow rate, q, to an environment containing both QSIs and antimicrobials.

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# **Proximal Point Approach for Moving Horizon Estimation: Real-Time Application to the Stabilization of a Double Inverted Pendulum**

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For the synthesis of feedback control law, full knowledge of all the state variables is required. This is not always possible as all state variables are, in general, not available for direct measurements. In this case, to apply state feedback, we must construct or obtain a good estimate of the state variables from available measurements. Among the many state estimation techniques discussed in the current literature is the Bayesian state estimation known as the Kalman filter [1]. Since its introduction in 1960, Kalman filter has been a subject of extensive research and has been applied to a wide range of applications, including navigation systems, financial and weather prediction, chemical plant control, and more recently, in the field of biomedicine. In its original form, the Kalman filter is a recursive formula that provides state estimation of a linear system. For nonlinear systems, one of the most widely used estimation algorithms is the extended Kalman filter (EKF). In the EKF, the nonlinearity of the system's dynamics is approximated through a linearization process around the last state estimate.

Moving horizon estimation (MHE) is another state estimation method that is useful for nonlinear or constrained dynamical systems. In MHE, recent measurements were used to find a trajectory of the state that fits the measurements most closely while minimizing the size of the modeling and measurement errors (see [2] and the references therein). In contrast to the Kalman filter, the state trajectory estimate is fit only to recent measurements (hence moving horizon) rather than the whole output history, though an additional term, called the arrival cost that penalizes the difference between the new and the last estimate, is included to ensure convergence and stability properties of the MHE algorithms.

The explicit minimization at each iteration of MHE can incorporate additional inequality constraints on state variables and measurement errors, providing advantages over Kalman filter for linear systems. For nonlinear systems, MHE has been demonstrated to outperform EKF in a number of cases. The disadvantage of MHE is the computational cost associated with solving a minimization problem at each iteration. In this talk, we will consider MHE within the framework of the proximal point minimization algorithm [3]. The effectiveness of the proximal point MHE strategy is then tested on the real-time state estimation for the stabilization of a double inverted pendulum on a moving cart.

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#### On the energy cascade of wave turbulence systems

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In weak turbulence theory, the Kolmogorov-Zakharov spectra is a class of time-independent solutions to the kinetic wave equations. In this talk, we construct a new class of time-dependent solutions to the initial value problems, with general initial conditions. These solutions exhibit the interesting property that the energy is cascaded from small wavenumbers to large wavenumbers. We can prove that starting with a regular initial condition whose energy at the infinity wave number  $p = \infty$  is 0, as time evolves, the energy is gradually accumulated at  $\{p = \infty\}$ . Finally, all the energy of the system is concentrated at  $\{p = \infty\}$  and the energy function becomes a Dirac function at infinity  $E\delta_{\{p=\infty\}}$ , where *E* is the total energy. The existence of this class of solutions is, in some sense, the first complete rigorous mathematical proof based on the kinetic description for the energy cascade phenomenon for waves with quadratic nonlinearities. We restrict our attention in this paper to the statistical description of acoustic waves. However, the technique is quite robust and can be applied to other types of wave turbulence kinetic equations. This is a joint work with Avy Soffer (Rugers).

# **Control of Bacterial Communities Using Deep Reinforcement Learning**

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Multi-species bacterial communities are widespread in natural ecosystems. Engineered synthetic communities have shown increased productivity over single strains and allow for the reduction of metabolic load by compartmentalising bioprocesses between multiple sub-populations. Despite these benefits, co-cultures are rarely used in practice because control over the constituent species of an assembled community has proven challenging. Here we demonstrate, in silico, the efficacy of approaches from artificial intelligence - reinforcement learning - in the control of co-cultures within continuous bioreactors. We first develop a mathematical model of bacterial communities within a chemostat that incorporates generalised Lotka-Volterra interactions. We then show that reinforcement learning agents can learn to maintain multiple species of cells in a variety of chemostat systems, with different dynamical properties, subject to competition for nutrients and other competitive interactions. Reinforcement learning was also shown to have the ability to maintain populations within more selective bounds, which is important for optimising the productivity of reactions taking place in co-cultures. Additionally, our approach was shown to generalise to systems of three populations and to be able to cope with random initial conditions. Three species systems represent a level of complexity that has not yet been tackled by more traditional control theory approaches. As advances in synthetic biology increase the complexity of the cellular systems we can build, the control of complex co-cultures will become ever more important. Data-driven approaches such as reinforcement learning will enable greater optimisation of environments for synthetic biology.

### **Ensemble-based Ultrahigh-dimensional Variable Screening**

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Since the sure independence screening (SIS) method by Fan and LV [1], many different variable screening methods have been proposed based on different measures under different models. However, most of these methods are designed for specific models. In practice, we often have very little information about the data generating process and different methods can result in very different sets of features. The heterogeneity presented here motivates us to combine various screening methods simultaneously. In this paper, we introduce a general ensemble-based framework to efficiently combine results from multiple variable screening methods. The consistency and sure screening property of proposed framework has been established. Extensive simulation studies confirm our intuition that the proposed ensemble-based method is more robust against model specification than using single variable screening method. The proposed ensemble-based method is used to predict attention deficit hyperactivity disorder (ADHD) status using brain function connectivity (FC).

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# On the numerical solution of advection-diffusion equations with singular source terms

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In this work, we present a numerical study for one-dimensional advection-diffusion equation having singular source terms. Singular in the sense that within the spatial domain the source is defined by a Dirac delta function. Solutions of such equations are typically non-smooth functions which forms an obstacle for standard numerical methods. A third order and a fifth order Weighted Essentially Non-Oscillatory (WENO) finite volume methods with non-uniform meshes [1] are used for the spatial discretization. As for the time discretization, we use the flux implicit Crank-Nicolson scheme [2]. Numerical examples are provided.

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### Investigation and Numerical Solution of the Discrete Analogue of Initial-Boundary Value Problem to One Nonlinear Parabolic Equation

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Investigation of some biological models bring us to the following initial-boundary value problem to nonlinear parabolic equation:

$$U_{t} = (k(x, t, U_{x})U_{x})_{x} + f(x, t, U), \quad (x, t) \in \Omega \times ]0, T], \tag{1}$$

$$U(0,t) = \phi_0(t), \quad x \in \Omega,$$
(2)  
$$U(0,t) = \phi_0(t), \quad U(1,t) = \phi_1(t), \quad t \in [0,T],$$
(3)

where U = U(x, t) is unknown function,  $k, f, \varphi, \phi_0$ , and  $\phi_1$  are given continuous functions, T = const > 0,  $\Omega = (0, 1)$ .

For the problem (1)-(3) we construct the following discrete analogue

$$\frac{u_{i}^{j+1}-u_{i}^{j}}{\tau} = \frac{1}{h} \left[ k \left( x_{i+1/2}, t^{j+1}, \frac{u_{i+1}^{j+1}-u_{i}^{j+1}}{h} \right) \frac{u_{i+1}^{j+1}-u_{i}^{j+1}}{h} - k \left( x_{i-1/2}, t^{j+1}, \frac{u_{i}^{j+1}-u_{i-1}^{j+1}}{h} \right) \frac{u_{i}^{j+1}-u_{i-1}^{j+1}}{h} \right] + f \left( x_{i}, t^{j+1}, u_{i}^{j+1} \right), \quad i = 1, 2, \dots, M-1, \quad j = 0, 1, \dots, N-1,$$

$$(4)$$

$$u_i^0 = \varphi_i, \quad i = 0, 1, \dots, M, \quad u_0^j = \phi_0^j, \quad u_M^j = \phi_1^j, \quad j = 1, 2, \dots, N,$$
 (5)

where  $hM = 1, \tau N = T$ ,  $\varphi_i = \varphi(x_i), i = 0, 1, ..., M, \phi_0^j = \phi_0(t^j), \phi_1^j = \phi_1(t^j), j = 1, 2, ..., N$ .

Under some restrictions on functions k and f we prove the theorem of comparison, theorems of existence and uniqueness of the solution of discrete analogue (4),(5). Also, for the discrete analogue (4),(5) we construct the iteration scheme and prove convergence of the iteration scheme to the solution of discrete analogue (4),(5). If solution U of the problem (1)-(3) is smooth enough, we also prove the convergence of the solution of discrete analogue (4),(5) to the solution of the problem (1)-(3).

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### **Recent Developments in 3D Sparse Grid Turbulence**

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The 3DS is a co-planar arrangement of grid elements, [1, 2, 3], Fig. 1, which reduces the maximum blockage ratio (solidity) of the grid system as compared to the 2D Regular Grid (RG) and 2D flat Fractal Grid (2DF),  $\sigma_{3DS}^{max} \ll \sigma_{2DF}$ . 'Sparse' is a reference to the spaces between co-frames that are free of grid bars. The 3DS possesses a bigger parameter space then the 2DF, the new parameters being the spacings between co-frames, the order of co-frame arrangement, and the blockage ratios of individual co-frames.

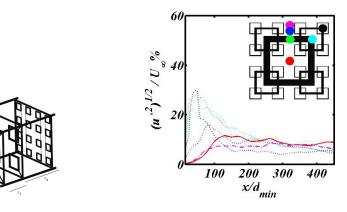


Figure 1: Example of 3DS grid pencils

Figure 2. Turbulence intensities in 3DS along streamwise

Here, we compare the turbulence generated by a 3DS grid ( $\sigma_{3DS}^{max} = 15\%$ ) with regular RG and 2DF grids ( $\sigma_{RG} = \sigma_{2DF} = 32\%$ ), reported in [4]. Simulations were carried out using DNS in a channel with aspect ratio 5:1:1 with inflow and outflow in the streamwise direction, and periodic conditions in the lateral directions. The Reynolds number based on the Kolmogorov scale  $d_{min} = 1$  was Re = 300. Although the overall development of the turbulence profiles in the 3-frame 3DS (15%) system are similar to the 2DF (32%) profiles in [4], the peak intensities in the 3DS is lower than in a 2DF system due to the lower blockage ratio, and the turbulence intensities in the 3DS is sustained far downsteam at a level comparable to the 2DF. Different blockage ratios and different order of co-frame arrangements yield markedly different peak intensities. This is important for future turbulence generation and control.

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## On the Solution of the Optimal Control Problem of Inventory of a Discrete Product in Stochastic Model of Regeneration

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The work considers a new complete model of discrete product inventory control in regeneration scheme with a Poisson flow of customer requirements and random delivery delay. In the system deferred demand is allowed, the volume of which is limited by a given value  $N_0$ . The control parameter r is the level of the stock, at which achievement it is necessary to make an order for replenishment, and this parameter is determined in accordance with a discrete probability distribution, which plays the role of a control strategy. The moments of change in the states of the regeneration process describing the functioning of the system are the moments of arrival of customers, if the value of deferred demand does not exceed the value  $N_0$ , and the moments of replenishment of the inventory.

As an indicator of control efficiency, we consider the average specific profit obtained during the regeneration period. In order to obtain an explicit representation for this indicator, a special version of the classical ergodic theorem [1] was proved for the additive cost functional, which has an additional component associated with regeneration moments. The optimal control problem is solved on the basis of the statement about the extremum of a fractional-linear integral functional on the set of discrete probability distributions [2]. It is established that the optimal control strategy is deterministic and is determined by the point of global extremum of the function, which is a stationary cost efficiency indicator and depends on the control parameter.

In the work, explicit representations are derived for the mathematical expectations of the increments of the profit functional on the regeneration period under all possible conditions on the control parameter, in other words, the decision taken on the specified period. These analytical representations enable us to explicitly obtain the stationary cost indicator of control efficiency as a function of the control parameter and, for given model characteristics, numerically determine the optimal value of the control, which contributes to solving one of the important applied problems of the modern economy.

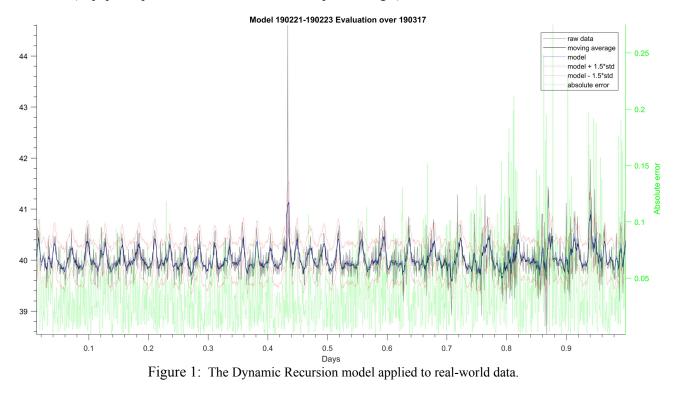
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# Dynamic Recursion (DR): A Multivariate Non/linear Autoregressive Model for Quasi-Periodic Signals

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Quasi-periodic signals / time series are ubiquitous in both scientific and industrial settings. An autoregressive model has been developed – a mathematical framework accompanied by a software package – in order to fill existing needs to model quasi-periodic signals arising in a wide range of applications, from optimizing energy usage in building science, through financial modelling, to satisfying supply logistics for maximizing profit. As such, it is an alternate take on problems often approached via more fashionable neural network models. The modelling task is an inverse problem, in the sense that it aims to find optimal parameters to fit the model to the data. The talk will present the theoretical model, and present computational results to demonstrate its practicality, while elaborating on mathematical questions pointing beyond the current heuristics. (A paper is planned to be submitted to the proceedings.)



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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 a 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 cracks. The piezoelectric strip being prescribed out-of-plane shear stress  $\tau_0$  and in-plane electric-displacement  $D_0$ . Consequently, under the combined electromechanical 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 zones are assumed to be of a negligible length, hence ignored. The developed saturation zones are 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 mathematical model framed of the above problem is solved using the 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 the length of developed saturation zones and fracture parameters {crack sliding displacement (CSD), crack opening potential drop (COPD), 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<sub>3</sub>, 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, COPD, IFs, LERR and GERR are presented graphically and compared.

From the numerical results, it is seen that cracks open more for the 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 is maximum for the impermeable case and minimum for the permeable case. For semi-permeable case, these fracture parameters lie between impermeable and permeable cases. This indicates that the electric permittivity of the medium inside the crack cannot be ignored.

Finally, all the graphical variations conclude that proposed model is capable to arrest the crack under smallscale electric yielding.

# Properties of the zeros of the scale delay equation $\dot{x}(t) = -ax(\alpha t)$ .

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The scale-delay system has been studied extensively. Valeev [2] showed that the scalar equation  $\dot{y}(t) = \mu y(t) + \beta y(\alpha t)$ , y(0) = 1, has a solution given by the series expansion

$$y(t) = 1 + \sum_{k=1}^{\infty} \frac{t^k}{k!} \prod_{i=0}^{k-1} (\mu + \beta \alpha^i),$$

and that this series has an infinite radius of convergence, hence is an entire function. He also showed that for  $\mu \neq 0$ , and  $0 < \alpha < 1$ , the solution diverges if  $|\beta| > |\mu|$  and converges if  $|\beta| < |\mu|$ . The special case,  $\mu = 0$ ,  $\beta = 1$  has the unit solution (y(0) = 1) (a.k.a. the deformed exponential)

$$y(t) = \sum_{k=0}^{\infty} \frac{\alpha^{k(k-1)/2}}{k!} t^k \stackrel{\text{def}}{=} E_{\alpha}(t),$$

which satisfies  $0 < y(t) < \exp(t^{\varepsilon})$  for all  $\varepsilon > 0$ , and  $y(t) \ge t^{\frac{\ln \ln t}{2\ln \alpha} + o(\ln t)}$ . With  $\mu = 0$  and arbitrary  $\beta$ , denote the unit solution by  $E_{\alpha}(\beta t)$ . The solution for  $\beta = -1$  is oscillatory and diverging. Its zeros are asymptotically given by  $t_k = \frac{k}{\alpha^{k-1}}(1 + \phi(\alpha)k^{-2} + o(k^{-2}))$ , where  $\psi(\alpha)$  is the generating function of the sum-of-divisors function  $\sigma(k)$  [5, 3]. Alternatively, it follows from Hadamard's factorization theorem that  $y(t) = \prod_{k=1}^{\infty} \left(1 - \frac{t}{t_k}\right)$ , where  $\{t_k\}$  are the roots of y. Zhabko et al. [4]' s extension showed that for  $\dot{x}(t) = Ax(t) + Bx(\alpha t)$ ,  $x \in \mathbb{R}^n$ , the system is asymptotically stable if  $\overline{\lambda} < 0$  and  $\overline{\mu} < 0$ , where  $\overline{\lambda} = \max_{f(s)=0} \operatorname{Re}\lambda$  and  $\overline{\mu} = \max_{\phi(s)=0} \operatorname{Re}\mu$  (setting  $\overline{\mu} = -\infty$  if there are no roots) and  $f(s) = \det(sI - A)$ ,  $\phi(s) = \det(A + e^{s\ln\alpha}B)$ . If  $\overline{\lambda} > 0$  or  $\overline{\mu} > 0$ , the system is unstable.

Consider the series of inverse powers of the roots of  $E_{\alpha}(-t)$   $S_n = \sum_{k=1}^{\infty} \frac{1}{t_k^n}$ , n = 1, 2, ... Denoting the coefficient of  $t^n$  in  $E_{\alpha}(t)$  by  $c_n$ , then the following recursion is known (see [1]) with  $S_0 = 1$ .

$$S_n + c_1 S_{n-1} - c_2 S_{n-2} + \dots + c_n S_0 = 0.$$

We show that these coefficients can be recursively computed, and give in particular the new sequential relations

$$S_{1} = 1$$

$$S_{2} = 1 - \alpha$$

$$S_{3} = (1 - \alpha)^{2}(2 + \alpha)$$

$$S_{4} = (1 - \alpha)^{3}(6 + 6\alpha + 3\alpha^{2} + \alpha^{3}).$$

In addition, the zeros satisfy  $\sum_{k=1}^{\infty} \frac{1}{\alpha t_k - t_\ell} = 0$ ,  $\ell = 1, 2, \dots$ 

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### **Combined Effect of Industrial Airborne Pollutants on Birth Outcomes in Alberta**

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Exposure to complex mixtures of industrial chemical emissions in the air poses a risk to our health, including the risk of the development of adverse birth outcomes (ABOs). Data mining is a useful tool to discover complex interactions between exposures in high dimensional data. We used association rule mining to identify relationships between combined airborne industrial chemical exposures and high ABO rates.

Data for births in the Canadian province of Alberta from 2006 to 2012 was obtained from the population based Alberta Perinatal Health Program (n=333,250) [1]. ABOs included small for gestational age (SGA, n=29,679), low birth weight at term (LBWT, n=22,733), and preterm birth (PT, n=5,485). Prenatal exposure to 136 registered industrial airborne chemicals was obtained using industrial emissions data reported by 6,279 Alberta facilities to the National Pollutant Release Inventory [2]. Wind pattern data from 182 stations in AgroClimatic Information System 2010 [3] was used to assess the mother's exposure to the chemicals.

Each birth and maternal exposure to a chemical(s) served as a "transaction" for the association rule mining. Association rules were mined using the Kingfisher algorithm [4]. We converted the lift to relative risk (RR), which does not depend on the exposure prevalence [5], and shortlisted the rules with  $RR \ge 1.5$ . The combinations of chemicals were then ranked based on their frequency of appearance in the shortlisted rules, as more frequent combinations may point to possible casual effects that worth future research.

There were a total of 10,788 "significant" rules, including 2,238 rules for SGA, 5,497 rules for LBWT, and 3,053 rules for PT. The most complex exposures included combinations of up to 8 chemicals. Among the rules with  $RR \ge 1.5$ , the most frequent chemical combinations included two to four chemicals among chromium (and its compounds), lead (and its compounds), aluminum (fume or dust), carbon disulphide, methanol, n-Hexane, and Xylene (mixed isomers). While co-emission of lead, methanol and n-Hexane were frequently observed, the emission of each of aluminum, chromium, carbon disulphide and Xylene was largely independent.

We used association rule mining to identify the most frequent combinations of chemicals that have strong association with ABOs. These combinations, especially for independently emitted chemicals, shall be further investigated for individual importance as well as their interactions.

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# Categorizing elliptic curves with rational 2 torsion in terms of the existence of integer points

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We continue work of ours [6] and Bennett [1] concerning the existence of integer points on curves with rational 2 torsion, and relate the existence to various problems in Analytic Number Theory [5] and Diophantine Analysis [4]. Numerous open problems will be discussed along with a status report using recent theorems that follow from the work of Wiles and others [2], [3] on the applications of Galois representations to ternary Diophantine equations.

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# Artificial Viscosity Joint Spacetime Multigrid Method for HJB-KFP System Arising from Mean Field Games

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Mean field game theory is a branch of game theory that studies the competitions among infinite number of players, where individual players have negligible influence to the system, and respond to each other in a statistical sense. Numerous applications of mean field games have been proposed. Examples include, but not limited to, micro or macro economics, sociology, engineering, urban planning, etc.

Mean field games can be formulated as a system of partial differential equations (PDEs) that consists of two equations. One equation is a backward Hamilton-Jacobi-Bellman (HJB) equation for the optimal value function of the players, denoted as u. The other equation is a forward Kolmogorov-Fokker-Planck (KFP) equation for the distribution (or density function) of the players' states, denoted as m. The two PDEs are nonlinear and coupled with each other. It is usually impossible to derive the solutions analytically. Hence, it is desirable to compute the numerical solutions.

Finite difference discretization gives rise to a nonlinear discretized system. The size of the nonlinear discretized HJB/KFP system can be large, which requires effective and fast solvers. In this talk, we propose a fast multigrid solver for the discretized HJB-KFP system. In contrast to the standard approach, our multigrid method is applied on the entire spacetime. To emphasize that  $(u_h, m_h)$  are solved together, we call this proposed approach "joint" spacetime multigrid method.

Moreover, standard multigrid components turn out to be ineffective for the discrete HJB/KFP system. We explore different novel techniques. First, the pointwise Gauss-Seidel smoother does not smooth errors on the time direction. To address this issue, we propose a hybrid of full and semi coarsenings. The time direction is coarsened only if errors on the time direction are smoothed. The other issue is that the coarse grid matrix using direct discretization is not accurate for convection dominated problems. Our idea is to add artificial viscosity to the direct discretization coarse grid operator in order to compensate for the error.

We apply Fourier analysis to illustrate the efficiency of our proposed multigrid method. Numerical experiments show that the convergence rate of the new multigrid method is mesh-independent and faster than the existing methods in the literature.



Figure 1: Dimensionless parameter x = 0.02, n = 100, (a) for linear-polarized light, (b) for circular-polarized light.

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### Quantum light and Topological surface states

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The light is a powerful tool to change the properties of materials, for example experiments have demonstrated that superconductivity can be induced through infrared pulses in high-temperature cuprate superconductors [1]. In recent years new states of quantum matter called 3D topological insulators appear. 3D topological insulators (TIs) were theoretically predicted to exist [2] and have been experimentally discovered [3], they are electronic materials that have a bulk band gap like an ordinary insulator but have protected conducting states on their surface [4]. The topological protection of their surface states, together with the spin-momentum locking due to the strong spin-orbit coupling, yields a variety of novel phenomena, such as the magnetoelectric effect, axion electrodynamics, and surface Hall effect [4]. Optically engineering of the topological band structure is in focus of attention [5], where the light field can be introduced by a periodic potential. As continuous time translational invariance is broken by the periodic potential, it is no longer appropriate to discuss energy eigenstates, but with the Floquet theory, the so called Floquet state and associated quasienergies can be defined and can be regarded in an analogous way to the eigenstates and corresponding energies of a static system [6], extending the time-independent topological classification. By using appropriate periodic driving field, a nontrivial topological band structure can be generated. In the Floquet theory approach, the TIs are treated as quantum systems, the field is treated classically.

In this talk, starting from a different approach that combines TIs and quantized electromagnetic fields, we find that the elementary excitations spectrum is dependent on the polarizations of quantum light. The article is organized as follows : the first part focuses on linear–polarized light, the second part is about circular–polarized light.

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# Symmetry, Hopf Bifurcation and Phase-Locked Solutions in Time Delayed Neural Networks

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We consider networks of N identical oscillators with time delayed, global circulant coupling, modeled by a system of delay differential equations with  $Z_N$  symmetry:

$$X'_{i}(t) = F(X_{i}(t), X_{i}(t-\tau_{s})) + \sum_{j=1}^{N} w_{ij} G(X_{i}(t), X_{j}(t-\tau)), \ i = 1, \cdots, N,$$
(1)

where  $X_i$  denotes the variables of a *m*-dimensional subsystems,  $\tau_s$  is the self-feedback delay, and  $\tau$  is the coupling time delay between different nodes. *F* and *G* are smooth functions that describe the internal and coupling behavior of the subsystems, respectively. The coupling matrix has the form  $W = (w_{ij}) = circ(w_0, w_1, \dots, w_{N-1})$ . Since we are primarily interested in applications in neuroscience we focus on coupling where the oscillators are coupled through their first variable.

We give explicit conditions on the nonlinearities of the model (1) for the existence of Hopf bifurcations induced by coupling time delay. We show, using symmetric Hopf bifurcation theory, that each delay induced bifurcation gives rise to an oscillatory solution with a particular type of phase-locking between the oscillators. Our general results are then applied to two example networks of neural oscillators and perturbation analysis is used to predict the criticality of the Hopf bifurcation. Example results are shown in Figure 1.

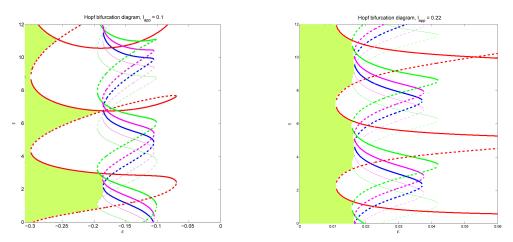


Figure 1: Delay-induced Hopf bifurcation curves for a network of six Morris-Lecar neurons. Each colour corresponds to a different type of phase-locking. Parameters are the coupling delay  $\tau$  and the coupling strength  $\varepsilon$ . In the yellow region the synchronous equilibrium point is asymptotically stable.

<sup>[1]</sup> Symmetry, Hopf bifurcation and the emergence of cluster solutions in time delayed neural networks. CHAOS 27(11) (2017) 114316.

# **Algorithms for the Multiplication Table Problem**

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Let M(n) be the function that counts the number of distinct integers in an  $n \times n$  multiplication table. That is,  $M(n) = |\{ij: 1 \le i, j \le n\}|$ . The asymptotic study of this function was initiated by Erdős [1] showing  $M(n) = o(n^2)$ and the current best known result is due to Ford [2]. He proved

$$M(n) \approx \frac{n^2}{(\ln n)^c (\ln \ln n)^{3/2}},$$
(1)

where  $c = 1 - \frac{1 + \ln \ln 2}{\ln 2} = 0.086071...$ 

We state algorithms and analyze their run-time and space constraints for single evaluation and tabulation of M(n). Single evaluation was initiated by Brent and Kung [3]. They used a straightforward modification of the sieve of Eratosthenes to evaluate M(n) in time and space  $O(n^2)$ . We give a new incremental algorithm that tabulates M(k) for all  $k \le n$  in time

$$O\left(\frac{n^{2}(\ln n)^{1-c}}{(\ln \ln n)^{3/2}}\right)$$
(2)

and requires only O(n) space. In practice, the incremental algorithm outperforms the straightforward version for the problem of single evaluation even though it has a worse asymptotic run-time. We describe a modification to this incremental method that can tabulate in time  $o(n^2)$ . Finally, we describe the computation that gave a tabulation of M(k) for  $k \le 2^{30}$ .

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## **Infinite Horizon Models of the Limit Order Book**

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We consider a bidding game, modeling a Limit Order Book (LOB) in a stock market. 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, while 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. Due to the competition, asking a higher price for an asset reduces the probability of selling it. Since each agent maximizes his expected payoff, a unique shape of the LOB is determined, which represents a Nash equilibrium.

Our more recent models account for the time-evolution of the LOB, assuming that the fundamental value of the stock varies stochastically. We study the optimization problem for each agent, in infinite-time horizon, exponentially discounted in time, and determine how the value function changes, depending on the modeling parameters.

# On the near-field cloaking problem for Maxwell's equations with passive stratified anisotropic media

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In this talk, I will discuss the near-field cloaking and associated inverse problem for Maxwell's equations with passive stratified anisotropic media using the electromagnetic "Dirichlet-to-Neumann" (DtN) map. As my primary interest is on fundamental limitations to practical cloaking devices, the focus is on frequency-dependent, lossy media (i.e., time-dispersive and dissipative). As a first step in this direction and building on previous work [1], I discuss the relevant algebraic and analytic properties of the DtN map (especially those pertaining to linear fractional transformations and Herglotz functions), and conclude with recent results for shell-type cloaking/inverse problems in one-dimensional layered media.

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### A Mathematical Model to Explore the Consequences of Inflammation in Cancer

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Inflammation is known to be a powerful promotor of tumour growth that is difficult to measure and quantify *in vivo*. Here I propose a mathematical model to explore the influence of inflammation on tumour growth, and to determine potential consequences it may have on treatment and metastasis. To begin, we use experimental data of simultaneous tumour growth at two distinct sites that exhibits a growth pattern of one large and one small tumour per mouse [1]. We hypothesize that unbalanced inflammatory cell accumulation may contribute to the growth rate separation in the data. To test this, we develop a mathematical model for tumour growth with inflammation and systemic competition between the two cancer sites. Using this predictive model, we explore the role of tumour-promoting inflammation in the observed growth rate differences. Due to the experimental setup, immune predation may be neglected, focusing the model on tumour-promoting immune actions only.

We use a multi-compartment differential equation-based model that assumes logistic growth for both the cancer and immune compartments. The carrying capacity of the tumour is dynamic and is described by a third differential equation. The model for one tumour is

$$\frac{d}{dt}C(t) = \alpha C(t) \left(1 - \frac{C(t)}{K(t)}\right)$$
(1)

$$\frac{d}{dt}K(t) = p(1+I(t))^{a}C(t)^{1-a} - qK(t)(1-I(t))^{b}C(t)^{\frac{2}{3}-b}$$
(2)

$$\frac{d}{dt}I(t) = \beta \left(I(t) + \rho C(t)\right) \left(1 - \frac{I(t)}{K_I}\right),\tag{3}$$

where C(t) is the cancer volume, K(t) is the cancer carrying capacity, and I(t) is the immune volume.

The model is parameterized by fitting to single-tumour experimental data using a simulated annealing algorithm. It is then extended to the two-tumour scenario by specifying the tumour site i, and linking the systemic immune response through the modified equation:

$$\frac{d}{dt}I_{i}(t) = \beta \left(I_{i}(t) + \rho C_{i}(t)\right) \left(1 - \frac{I_{1}(t) + I_{2}(t)}{K_{I}}\right), \quad \text{for } i = 1, 2$$
(4)

Numerical simulations are used to explore potential mechanisms driving the growth rate separation of the two tumours. The model predicts that unbalanced inflammatory actions, and in particular, a pre-inflamed site, can cause the growth disparities observed in the experimental data. This adds another potential mechanism contributing to the concomitant resistance observed in the data. The model is then used to explore potential consequences of inflammation on metastasis post surgery, when inflammatory conditions are altered.

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# Finite element modelling and simulation tools for investigation of the process and materials 3D-printed by Selective Laser Melting

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Selective Laser Melting (SLM), like many other additive manufacturing techniques, offers flexibility in design expected to become a disruption to the manufacturing industry. The current cost of SLM process does not favor a try-and-error way of research; which gives more room for modelling and simulation in that field of research. In this work we present a full model using Finite Elements Methods to solve a multi-scan SLM process problem. In the model, a combination of Ray-Tracing technique, a solution of the Radiation Transfer Equation and absorption measurements is used to establish an analytical equation that gives a more accurate approximation of laser energy deposition in powder-substrate configuration. With the new energy deposition model, other physics involved in the process are carefully set as well. These include the heat transfer equation in both solid and liquid parts of the system, different heat flux boundary conditions, laminar flow in the molten pool, recoil pressure during vaporization, volume forces and Marangoni effect. The adjusted model is able to produce reliable cooling curves and melt truck geometry that link well with experimental observations. One of the applications is the use of simulated tempering parameter, from Holloman-Jaffe equation, to investigate the martensitic inclusion across the printed part and match it with local micro hardness.

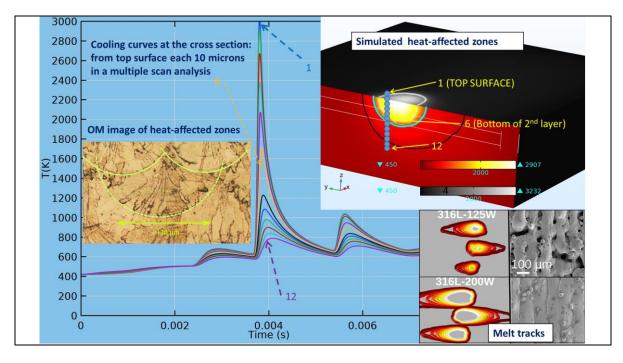


Figure 1: Simulated heat-affected zone, cooling curves, melt pool tracks and their experimental counterparts.

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# **Inferring Rankings From First Order Marginals**

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Motivated by applications in ranked-choice voting, we consider the problem of recovery of election results encoded by a function f on the symmetric group—given only partial data. In particular, we investigate the combinatorial structure of the matrix of first order marginals, which gives the number of voters who ranked each candidate in each position. We investigate conditions on f that allow us to exploit this combinatorial structure to recover the original function f. A relaxation of these conditions leads to the additional question of determining families of functions that share the same matrix of first order marginals. We investigate shared voting theoretic properties, for example, Condorcet winners, within these families of functions. As the matrix of first order marginals is the Fourier coefficient of the permutation representation of the symmetric group, this work sits within the context of algebraic compressed sensing, which tackles the question of how to recover a sparse function f on a finite group given only a subset of the Fourier coefficients of f.

# A Framework for Data-Driven and Compute-Intensive Applications on High Performance Computers

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We present a workflow framework which facilitates data-driven and compute-intensive applications to run on a cluster of high performance computer. The Distributive Interoperable Executive Library (openDIE [1]) framework combines popular machine learning tools and traditional parallel physics and engineering programs, giving users an easy tool to explore the emergent modeling method of data-assist simulations for a wide variety of applications. OpenDIEL is a workflow engine that aims to give researchers and users of high performance computing (HPC) an efficient way to coordinate, organize, and interconnect many disparate modules of computation in order to effectively utilize and allocate HPC resources. A GUI is provided to create workflows, and allows for the specification of data science jobs, including specification neural network architectures, data processing, and hyperparameter tuning. Existing machine learning tools can be readily used in the openDIEL, allowing for easy experimentation with various models and approaches.

We also introduce a new machine learning tool called MagmaDNN [2] which is fully integrated to openD-IEL and is designed to scale on supercomputers equipped with GPUs. It derives its performance power from the MAGMA [3] library, a set of linear algebra routines for HPC platforms and GPUs. MagmaDNN, uses well established HPC techniques such as task-based parallelization, DAG representations, scheduling, mixed precision algorithms, asynchronous solvers, and autotuned hyperparameter optimization. We will illustrate these techniques and their incorporation and use comparing to other frameworks, currently available.

In this paper, we will present the integrated functionality of openDIEL with usecases in MagmaDNN. Benchmark results of a materials science applications and a traffic flow application will also be presented.

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# **Impulsive Distance-based Formation Tracking Control of Multi-agent Systems**

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In this paper, we discuss the distance-based formation tracking problems for double-integrator multi-agent system (MAS) via impulsive protocols. The impulsive algorithms are designed by using the relative distance information of the neighbors. The proposed controller allows all agents to both achieve the desired shape and reach the same velocity with moving leader by controlling the distances and velocities.

In the existing literature, many different continuous control methods have been utilized including the adaptive control, feedback control and so on (see Refs. [1]). Unlike the continuous control method, the impulsive control is only exerted at impulsive instants, which is more reasonable and applicable to add a jump to the state of agents (see Refs. [2][3]). For the continuous control part, we will generate a general potential function and use relative distance information of inter-agents to form and keep the desired formation shape. While at every moment  $t_k$  we apply an impulsive control to velocity. By using Lyapunov's second method, the asymptotic stability of the system with the proposed impulsive control law has been demonstrated. Numerical examples are provided to validate the effectiveness of our approach.

The main contribution of this paper can be summarized as follows.

- 1. An impulsive algorithm is designed for distance-based formation tracking problem with a general gradient function term and the impulsive gains. By introducing a virtual leader into our model, we address the problem of motion and formation control as a whole.
- 2. Based on the Lyapunov's second method, the asymptotic stability of the double-integrator MAS with a leader under the proposed distributed impulsive controller is achieved.
- 3. The sufficient conditions are derived for the distance-based formation tracking of the MAS. These results give the guidelines to design the impulsive formation tracking algorithm for the double-integrator MAS.

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Title: Central configurations in planar 6-body problem forming two equilateral triangles

Speaker: Zhifu Xie Affiliation: The University of Southern Mississippi

A Central Configuration (CC) is a special arrangement of masses in the \$n\$-body problem where the gravitational force on each body points proportionally toward the center of mass. A stacked CC is a CC that has a proper subset of the \$n\$ bodies also forming a CC. In this paper, six bodies are located on two equilateral triangles \$\Delta\_{123}\$ and \$\Delta\_{456}\$. Assume that both triangles are symmetrical about the line connecting \$m\_3\$ and \$m\_4\$. Within these configurations, the six body configuration is not a central configuration if the triangle \$\Delta\_{123}\$ is above or below the triangle \$\Delta\_{456}\$. It is also not a central configuration if more than two of the six bodies are collinear. When the two equilateral triangle configurations have a common centroid, masses on each equilateral triangles must be same respectively and the configuration can form a central configuration only if the ratio of the lengths of the sides between \$\Delta\_{123}\$ and \$\Delta\_{456}\$ falls into certain ranges. Moreover there are some numerical evidences that, first there are exactly two nested central configuration but there may be one, two, or three twisted nested CC for a given mass ratio; and second, there exists central configurations other than same centroid.

# Input-to-State Stability of Coupled Reaction-Diffusion Neural Networks: Delay-Dependent Pinning Impulsive Control

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Recent years have witnessed the great progress in the input-to-state stability analysis of coupled neural networks. Numerous studies have been reported by utilizing various kinds of control methods. Among them, the impulsive control and pinning control have been proved to be effective to reduce the computing cost and achieve input-to-state stability of coupled neural networks. However, most of the results have not considered the time delays existed in the impulsive controller, and very few works about the pinning impulsive control with distributed delay have been reported in the literature[1, 2].

This paper studies the input-to-state stability of coupled reaction-diffusion neural networks with time-varying delays. A novel pinning impulsive controller is proposed, where distributed delays and discrete delays are taken into account, respectively. By using the Lyapunov-Krasovskii method, we derive sufficient conditions on the system parameters, impulsive gains, pinned node numbers, impulsive instants and time delays. input-to-state stability criteria are established for the delayed coupled reaction-diffusion neural networks. Our results show that input-to-state stability prosperities can be guaranteed by controlling a small portion of nodes in the networks via delayed impulses. Numerical examples are provided to demonstrate the effectiveness of the theoretical results.

The main contributions of this paper are given in the following three aspects:

- 1. A more general pinning impulsive algorithm is designed to guarantee the input-to-state stability of the coupled reaction-diffusion neural networks, in which the pinned node number and the impulsive gains are impulsive-instant dependent, i.e., at distinct impulsive instants, the number of pinned nodes and the impulsive gains are different.
- We introduce a type of Lyapunov-Krasovskii functional candidates, which consist of a function part and a functional part. Based on the Lyapunov-Krasovskii functionals, input-to-state stability of reaction-diffusion neural network with distributed-delayed impulses and discrete-delayed impulses are achieved, respectively.
- 3. Appropriate inequalities are developed to derive sufficient conditions for input-to-state stability of reactiondiffusion neural networks.

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# A within-host model of influenza A (H9N2) virus infection dynamics and type-I interferon response in chickens

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Within-host mathematical modeling can improve our understanding of disease dynamics and help to inform intervention strategies [1]. Low pathogenic H9N2 avian influenza (AI) is a zoonotic pathogen which has significant economic and agricultural impact, but research on H9N2 AI virus kinetics in chickens is limited. A better understanding of the host innate immune response, which plays a crucial role in reducing viral shedding in chickens may contribute to the development of improved poultry vaccines and vaccination protocols. The study objectives were to use a within-host model to determine the impact of three type-I interferon (IFN) antiviral response pathways and a cellular latent period on cloacal and respiratory virus shedding in chickens. A deterministic compartmental model of target and infected host cells, type-I IFN response, and virus particles was developed. The model was parameterized using least squares fitting to H9N2 virus shedding titres from experimentally infected chickens [2]. The three type-I IFN pathways assessed included the reduction of virus replication in infected cells, induction of a non-susceptible cell state, CD8<sup>+</sup> T-cell destruction of infected cells (IFN pathways 1-3, respectively). The impact of a cellular latent period was evaluated using an eclipse phase compartment to represent infected cells which are not yet producing virus. The best-fit model was determined using the corrected Akaike Information Criterion. The model demonstrates that the inclusion of type-I IFN pathways 1 and 3 with an eclipse phase was most consistent with experimental cloacal virus shedding, while respiratory virus shedding was best simulated by an eclipse phase model which accounts for type-I IFN pathway 1 only. Viral infection of gastrointestinal (GI) cells leading to cloacal shedding also showed increased virus production and sensitivity to type-I IFN response compared to infection in respiratory cells. An eclipse phase of 7 and 17 hours were best able to simulate virus shedding in both gastrointestinal and respiratory infections, respectively. These results demonstrate potential differences between H9N2 AI infections in respiratory and GI cells, and the impact of an eclipse phase on time to peak virus shedding.

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#### **High-Frequency Statistical Modelling for Jump-Diffusion Asset Price Processes**

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We consider a multivariate jump-diffusion process to model the dynamics of multiple assets along with a systemic behaviour of the whole financial market. We assume that the S&P 500 stock index can be used to describe the systemic dynamics of a financial market. The model is similar to the jump-diffusion model proposed in [1] for modelling financial securities that have missing or asynchronous data in time series of historical prices. The model is constructed in such a way that all assets correlate with each other only implicitly through the systemic process. To calibrate the model, we first estimate parameters of the systemic asset and then estimate parameters for each other asset by conditioning on the parameters of the systemic asset. The multinomial maximum likelihood estimation method [2] can be employed. The proposed asset price processes have the following form:

$$S_0(t) = S_0(0) \times \exp\left\{ (\mu_0 - \frac{\sigma_0^2}{2})t + \sigma_0 \left( W_0(t) + \sum_{j=1}^{N(t)} Q_j \right) \right\},\tag{1}$$

$$S_{i}(t) = S_{i}(0) \times \exp\left\{\left(\mu_{i} - \frac{\sigma_{i}^{2}}{2}\right)t + \sigma_{i}\sqrt{1 - \rho_{i}^{2}}W_{i}(t) + \sigma_{i}\rho_{i}\left(W_{0}(t) + \sum_{j=1}^{N(t)}Q_{j}\right) + \sum_{k=1}^{N(t)}Q_{k}^{(i)}\right\},$$
(2)

where  $S_0$  is the value of a market index, and  $S_i$  with  $i \ge 1$  is the price of the *i*th asset. Here, Brownian motions  $\{W_0\}$  and  $\{W_i(t)\}$ , Poisson processes N(t) and  $N_i(t)$ , and sequences of jump sizes  $\{Q_j\}$  and  $\{Q_k^{(i)}\}$  are jointly independent.

In our research, we analyze if the systemic component can explain all jumps in the market dynamics. That is, all jumps are synchronized, and the asset price process  $S_i$  has no independent jump component. The alternative hypothesis is that there are disjoint jumps. We use the modelling approach and the statistical approach. First, we calibrate and compare two models: the model with co-jumps only and the model with both co-jump and independent jump components. The Kolmogorov–Smirnov test is used to compare the models. Secondly, we use jump tests to detect disjoint jumps in inter-day time series of asset prices. There are two approaches. One method is to remove the systemic component, create a new time series of asset price and then apply the Aït-Sahalia and Jacod jump test [3] to see if it has jumps or not. The second method is to use Jacod and Todorov's disjoint jump test [4] on the given high-frequency multi-asset time series directly, to see whether the systemic component from the S&P 500 stock index is able to explain all jumps.

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# **Discontinuous Galerkin method for a two-dimensional fractional reaction-diffusion equation from combustion process**

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In this talk, a two-dimensional temporal fractional combustion model with Caputo derivative is considered. We design an ingenious adaptive finite difference discontinuous Galerkin method to solve this model. To catch quenching moment more accurately, an explicit bisection adaptive strategy is proposed for discretization of fractional derivative. Discontinuous Galerkin method is employed for spatial discretization to settle large gradient changes and non-smoothness property of solution in adjacent area of quenching moment. The physical properties of combustion process, such as positivity, monotonicity, are theoretically or numerically investigated. Finally, we carry out systematic numerical experiments for such abstract combustor with different shapes and various parameter settings, which illustrate that the dynamics of such model depends on the intensity of initial inputs, the order of fractional derivative and the area of spatial domain.

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#### **Error Estimation for Fan Beam Algorithm**

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*Abstract*—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 Back-projection algorithm with window function is an approximation algorithm. This script defines a convolution back-projection algorithm at the discrete points on the X-rays passes through the objects. As the projection points are only lattice points, the back-projection is applied on that lattice points which reduces the original projection set in classical Radon transform. But this data point provides comparable results for fan beam geometry as the continuous geometry dispense to us. 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 more efficient than parallel beam projection.

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

In this formula of error analysis, approximation function is converging for larger values of both band-limit b and D (distance between source and origin of reconstruction region). As we fix b and derivative value of 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. Thus compare to parallel case which depends on  $\frac{1}{b^2}$ , in fan beam case algorithm has less error with both the factors i.e.  $\frac{1}{(bD)^2}$ .

Keywords: Computed tomography, Convolution back-projection, Radon transform, Fan beam.

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## **Rigorous proof of existence and computation of a family of solutions in state-dependent delay equations**

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Given an analytic two-dimensional ordinary differential equation  $\frac{dx}{dt}(t) = X_0(x(t))$ , which admits a limit cycle, we consider the singular perturbation of adding a state-dependent delay:

$$\frac{dx}{dt}(t) = X(x(t), \varepsilon x(t - r(x(t)))), \qquad 0 \le \varepsilon \ll 1.$$
(1)

We show that for small enough  $\varepsilon$ , there exist a limit cycle and a two-dimensional family of solutions to the perturbed state-dependent delay equation (1), which resemble the solutions of the unperturbed ODE. More precisely, we find a parameterization of the limit cycle and its stable manifold for the perturbed equation.

Our work consists of two parts. In the theoretical part, we analyze the parameterization, and find functional equations to be satisfied (invariance equations). We prove a theorem in "*a posteriori*" format, that is, if there are approximate solutions of the invariance equations, then there are true solutions of the invariance equations nearby (with appropriate choices of norms). In the numerical part, we implement an algorithm which follows from the constructive proof of above theorem. See below for some numerical results:

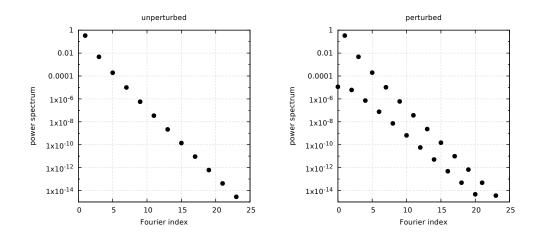


Figure 1: Power spectrum of the 1<sup>st</sup> component of the limit cycle for unperturbed and perturbed Rayleigh oscillator with  $\varepsilon = 0.01$ .

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## Stabilization for delayed stochastic systems with semi-Markovian switching and actuator saturation

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Due to the physical constraints of actuator, the actuator can only deliver control signals of limited magnitudes and rates, which makes actuator saturation inevitable in practice. In recent years, there have been many available references with respect to controller design for Markovian jump systems (MJSs) subject to actuator saturation, see, e.g. [1, 2, 3, 4] and references therein. However, to the best of our knowledge, up to now, there are few works on the stabilization for semi-Markovian jump systems (S-MJSs) with the effects of time-delay, stochastic disturbances and actuator saturation owing to its complexity and mathematical difficulty.

In this paper, the asymptotic stabilization problem for a class of delayed stochastic systems with semi-Markovian switching and actuator saturation is investigated. By applying the functional Itô's formula, multiple Lyapunov functionals and binary diagonal matrices, sufficient conditions for the local asymptotic mean square stability of the considered systems are established. Meanwhile, the mode-dependent state feedback controller and estimation of the domain of attraction in mean square sense are proposed in terms of linear matrix inequalities (LMIs). Finally, an example is given to illustrate the effectiveness of the proposed results.

The main contributions of this paper can be summarized as follows:

(1) The mode-dependent state feedback controller is designed for delayed stochastic S-MJSs with actuator saturation, which renders a more general model differing from S-MJSs without the effects of time-delay, stochastic perturbations and actuator saturation.

(2) Both stabilizable and unstabilizable subsystems are considered, which makes our results more practical.

(3) By using the functional Itô's formula, multiple Lyapunov functionals and binary diagonal matrices, a novel controller design method is proposed in terms of LMIs. Thanks to using path-wise derivatives, it is not necessary to conduct tedious derivation of the derivative formula for each specific sub-Lyapunov functional. Besides, with the help of binary diagonal matrices, we reduce the number of extreme realizations required to check feasibility without introducing conservatism.

(4) The local asymptotical mean square stabilization and estimation of the domain of attraction in the mean square sense are discussed.

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## Numerical PDE Methods for a Discontinuous Diffusion Problem with Application to Brain Cancer Growth

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Error analysis and convergence results for standard Partial Differential Equation (PDE) discretization methods normally assume that the coefficient functions are continuous. However, when the discretization methods are applied to PDEs (Boundary Value Problems - BVPs or Initial Value Problems - IVPs) with discontinuous coefficients, they may not exhibit the standard rate of convergence, and, even more, convergence is not guaranteed. In this research, we study a mathematical model simulating the invasion of brain cancer (glioma) which involves a PDE with discontinuous diffusion coefficient due to the heterogeneous nature of the brain, consisting of white and grey matter. The discontinuity of the diffusion coefficient results in continuity for the solution function, and a certain type of discontinuity of its spatial derivative, across the interface between the white and grey matters. We propose two approaches to adjust the standard Finite Difference methods, so that the numerical solution satisfies the continuity and discontinuity constraints. One technique treats the PDE as multi-domain problem with (interior) interface conditions forcing the continuity and discontinuity conditions either directly or through an integrationbased formulation of the PDE. The other relates the limits of the functional and forcing terms from both sides of the interface point. Numerical results will be provided to assess and compare the performance of the proposed methods.

## First Principle Calculations of Cobalt doped Cadmium Sulphide for Spintronics Applications

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By applying first principle calculation (DFT), we investigated the electronic, optical and magnetic properties of cobalt doped cadmium sulphide. Cobalt was doped in cadmium sulphide in different concentrations (0.0625 %, 0.1250 %, 0.1875 % and 25 %). In optical properties, the optical conductivity, absorption, reflectivity, dielectric constant, extinction constant and refractive index of Co doped cadmium sulphide were studied. Electronic properties of the material were also examined by discussing band gap and the band structure (bandgap), explained by density of states (DOS). Results were compared with the pure cadmium sulphide and it was observed that the Co doped CdS was semiconductor in the spin up channel and metallic in the spin down channel which showed the half metalic semiconductor nature of the Co doped CdS. Moreover, Magnetic moments were observed after the Co doping in CdS and it was observed that ferromagnetic character became strong in the material when the doping concentration increased up to 25% as compared to the other doping concentrations. Charge density of cobalt doped cadmium sulphide was also discussed and ionic character was found to be more powerful after doping. All these investigations were done by full potential linearized augmented plan waves (FP-LAPW) by utilizing Wien 2k code.

## Effects of Quality and Probabilistic Lead Time on the Optimal Production Lot Size and Supplier Selection

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This paper examines a production process in which a certain type of components is used in the production of the finished product. The components can be partially or fully acquired from any of *N* available suppliers. It is assumed that a single component is needed for the production of a single item of the finished product. Also, the components are received from the various suppliers in lots that contain some imperfect quality items. The percentage  $\gamma_j$  of imperfect quality components in a lot received from supplier *j*,  $1 \le j \le N$ , is random variable having known probability density function  $f_j(\gamma_j)$ . A 100% screening process conducted at the start of the production cycle is used to detect the imperfect quality components. These components are sold at the end of the screening period at a salvage price which is less than their purchasing cost.

A mathematical model is formulated to determine the optimal production lot size and supplier selection. Hence, the decision variables are the production lot size *y* and the proportions  $\pi_1, \pi_2, \ldots, \pi_N$  of the required components ordered from the *N* available suppliers. In addition to the quality of components, the mathematical model takes into account the probabilistic lead times of orders received from the suppliers. The lead time  $L_j$ , the time between placing and receiving the order from supplier *j*,  $1 \le j \le N$ , is random variable having known probability density function  $g_i(L_j)$ .

Expressions for the optimal lot size and the optimal selection of suppliers are derived using the formulated mathematical model. These expressions are shown to depend on the expectations of functions of the independent random variables  $L_1, L_2, ..., L_N$  and the independent random variables  $\gamma_1, \gamma_2, ..., \gamma_N$  (see Refs. [1, 2]). The optimal production lot size  $y^*$  and the optimal proportions  $\pi_1^*, \pi_2^*, ..., \pi_N^*$  of the required components ordered from the *N* available suppliers are shown to solve a constrained optimization problem that seeks to maximize the total profit per unit time function. An iterative algorithm is developed to numerically determine the optimal production lot size  $y^*$  and the optimal proportions  $\pi_1^*, \pi_2^*, ..., \pi_N^*$ .

Using suitable probability distributions identified in the literature for the quality of components (see Refs. [1, 2]) and lead time (see Refs. [1, 3]), numerical examples illustrating the calculations of the optimal solution and the selection of suppliers are provided. By incorporating the effects of quality and probabilistic lead time into the widely researched economic lot size model, the modeling approach presented in this study describes a practical production/inventory situation that resembles circumstances encountered in real life. This study adds to the extant literature on supplier selection and to the stream of research studies that have been conducted in the past two decades on incorporating quality into the classical production/inventory models. It provides managers and engineers with a practical model and an algorithm that enable them to make decisions that optimize their production operations and supplier selection.

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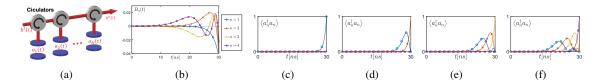


Figure 1: The setup(a) and the rotating frame wave function of orthogonal TMs (figure b) for a time-independent array of resonators with  $\kappa_0 = 1ns^{-1}$ , and the corresponding dynamics of the array upon their entry (figures c, d, e, and f).

#### Demultiplexing of photonic temporal modes by a linear system

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Single photon is an excellent carrier of quantum information, since its couplings to environments are very weak. There are numerous ways of encoding information with photon states, for example, encoding information in polarizations [1]. However, these methods can only encode very limited information in each photon, usually it is only one qubit due to the small Hilbert space.

Temporally and spatially overlapping but field-orthogonal photon temporal modes (TMs) that intrinsically span a high-dimensional Hilbert space are recently suggested as a promising means of encoding information on photons. Presently, the realization of photonic TM technology, particularly to retrieve the information it carries, i.e., demultiplexing of photonic TMs, is mostly dependent on nonlinear medium and frequency conversion. Meanwhile, its miniaturization, simplification, and optimization remain the focus of research. In this talk, we will propose a scheme of TM demultiplexing using linear systems consisting of resonators with linear couplings. Specifically, we examine a unidirectional array of identical resonators with short environment correlations. For both situations with and without tunable couplers, propagation formulas are derived to demonstrate photonic TM demultiplexing capabilities. The proposed scheme, being entirely feasible with current technologies, might find potential applications in quantum information processing.

The setup is illustrated in Fig.(1(a)) and the results are show in other figures of Fig.(1). Note that demultiplexers for a wide range of sets of orthogonal TMs can be engineered by altering the tunable coupling and allowing different resonators to have different functions of tunable coupling. For unidirectional array and with a given set of orthogonal TMs, an obvious approach to find the tunable coupling function is to use a sequential iteration of zero dynamic principle on each resonator under single excitation scenario.

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## Sustainable finance: a model of real-financial sector interaction, behavioural cycles, and the role of proactive supervision and risk management

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Collective action problems and the need for coordinated decision-making are at the heart of many contemporary global challenges, such as climate change, economic inequality, and systemic risk in the financial system. We ask, under what conditions do people succeed (or fail) to coordinate their individual behaviours in order to achieve a collectively sustainable outcome, and to protect themselves from large systemic breakdowns? The prevention of systemic risk has characteristics of a public good, and tends to be underprovided by risk-seeking market actors as memories of a past financial crisis fades.

Using a nonlinear system of ordinary differential equations, I draw from the existing literature to build a macroeconomic model of real-financial sector interaction. This features the relations between banks, firms and households, including banks' capital and leverage, the accumulation of private sector debt, and the possibility for debt defaults.

We model banks' changing behaviour within a returns- and market-share-driven environment. Besides their traditional loan and deposit business, banks can choose to boost returns with increased trading activity during a period of rising asset prices. Trading activity may be fuelled by off-balance sheet financial innovation. Banks are internally divided between the growth priorities of the "front office" and the risk management and monitoring priorities of the "back office" and bank supervisory authorities. Sustainable banking requires balance between the two.

Assuming that financial innovation is ongoing, and taking the endogenous instability of the financial system as given, our model asks, to what extent do institutions that promote prudential norms and rulecompliance succeed at dampening the severity of downturns?

One approach to lean against banks' pro-cyclical myopia through the cycle has been advocated in common by thinkers as diverse as economist Hyman Minsky, banking expert Moorad Choudhry, and former regulator John Palmer: they recommend monitoring banks' balance sheets, and limiting banks' leverage ratios and dividend payout ratios as prudential tools to constrain behaviour.

### **Deterministic Production of More Than 10000 Atom Entangled Dicke State**

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Since they were introduced by Dicke in an effort to explain superradiance in 1954, Dicke states have attracted widespread attention. In recent years, they have also found potential applications in quantum information science and precision measurement. For instance, they can be used to achieve measurement precision beyond the classical limit, or the standard quantum limit (SQL). Using N independent or uncorrelated particles, such as photons or atoms, the achievable precision for two-mode (or two-path) interferometry is bounded by the SQL,  $1/\sqrt{N}$ . Despite being a challenging benchmark, SQL has been approached in a number of systems, including LIGO and today's best optical atomic clocks. Precision beyond the SQL can be achieved by using entangled states such as Dicke states mentioned above so that quantum noises from individual particles null out, and in the ideal case, Heisenberg limit (HL) precision, 1/N, can be reached.

This work reports our successes in deterministic generations of (balanced) pseudo-spin-1/2 [1] and spin-1 [2] Dicke states of more than 10000 atoms in an atomic condensate, making use of controlled quantum phase transition (QPT) by crossing near adiabatically over QPT points in a spin-1 Bose-Einstein Condensate of <sup>87</sup>Rb atoms. We calibrate their non-classical properties and benchmark their interferometric performances in terms of state rotation measurement precisions beyond the SQL.

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#### Decoys and dilution: the impact of incompetent hosts on prevalence of Chagas disease

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Biodiversity is commonly believed to reduce risk of vector-borne zoonoses. This study focuses on the effect of biodiversity, specifically on the effect of the decoy process (additional hosts distracting vectors from their focal host), on reducing infections of vectorborne diseases in humans. Here, we consider the specific case of Chagas disease and use mathematical population models to observe the impact on human infection of the proximity of chickens, which are incompetent hosts for the parasite but serve as a preferred food source for vectors. We consider three cases as the distance between the two host populations varies: short (when farmers bring chickens inside the home to protect them from predators), intermediate (close enough for vectors with one host to detect the presence of the other host type), and far (separate enclosed buildings such as a home and hen-house). Our analysis shows that the presence of chickens reduces parasite prevalence in humans only at an intermediate distance and under the condition that the vector birth rate associated with chickens falls below a threshold value, which is relative to the vector birth rate associated with humans and inversely proportional to the infection rate among humans.

## Ebola: Impact of hospital's admission policy in an overwhelmed scenario

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Infectious disease outbreaks sometimes overwhelm healthcare facilities. A recent case occurred in West Africa in 2014 when an Ebola virus outbreak overwhelmed facilities in Sierra Leone, Guinea and Liberia. In such scenarios, how many patients can hospitals admit to minimize disease burden? This study considers what type of hospital admission policy during a hypothetical Ebola outbreak can better serve the community, if overcrowding degrades the hospital setting. Our result shows that which policy minimizes loss to the community depends on the initial estimation of the control reproduction number,  $R_0$ . When the outbreak grows extremely fast ( $R_0 \gg 1$ ) it is better (in terms of total disease burden) to stop admitting patients after reaching the carrying capacity because overcrowding in the hospital makes the hospital setting ineffective at containing infection, but when the outbreak grows only a little faster than the system's ability to contain it ( $R_0 \gtrsim 1$ ), it is better to admit patients beyond the carrying capacity because limited overcrowding still reduces infection more in the community. However, when  $R_0$  is no more than a little greater than 1 (for our parameter values, 1.012), both policies result the same because the number of patients never exceeds the maximum capacity.

### Developing a numerical model to predicting desalinated water production from the humid atmosphere by underground condensation

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One of the new methods of water production in low capacities is the use of air humidity, which is known as condensation water production and condensation irrigation system [1]. In this method that illustrated in fig1, the hot and humid air flow directed to the buried pipes in the ground, then the air is gradually cooled down and the vapor contained therein appears as drop-lets of water on the pipe surface [2]. The assessment of the amount of water extraction in the condensation system of hot and humid air is the main objective of this research. In this research, the governing equations on the problem, its boundary conditions and the initial conditions for a condensation water production sample system are extracted and explain using a finite volume method. Then, by developing a computer code and modeling in MATLAB software, the amount of water extracted from air humidity in buried pipes in depth of half a meter for different lengths was predicted and optimal pipe length in these systems was introduced. The numerical results show that in a 25 m long pipe with a diameter of 0.2 m, input air temperature of 50°C, soil temperature of 26 °C, relative humidity of 100% and air speed of 3.5 m/s, daily water production rate will be 1 kg per day. Also, the influence of effective parameters on the performance of the condensation water production system, including temperature and humidity of inlet air, soil temperature and inlet air velocity, have been evaluated. It was found that the results of numerical model are compatible with the experimental data of previous research [3].

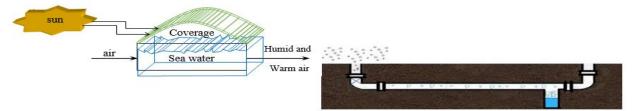


Figure 1- A schematic of how water is condensed from humidity

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## Large Time Behavior of Logarithmic Keller-Segel-Fisher/KPP System

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We consider the Keller-Segel-Fisher/KPP chemotaxis model with logarithmic sensitivity and logistic growth:

$$\begin{cases} s_t = \varepsilon s_{xx} - \mu us - \sigma s, \\ u_t = Du_{xx} - \chi [u(\ln s)_x]_x + au(1 - \frac{u}{K}), \end{cases} \qquad x \in \mathbb{R}, \quad t > 0.$$

$$(1)$$

Here the unknown functions are s = s(x,t) and u = u(x,t) for the concentration of a chemical signal and the density of a cellular population, respectively. The system parameters are interpreted as follows:  $\varepsilon \ge 0$  is the diffusion coefficient of chemical signal;  $\mu \ne 0$  the coefficient of density-dependent production/degradation rate of chemical signal;  $\sigma \ge 0$  the natural degradation rate of chemical signal; D > 0 the diffusion coefficient of cellular population;  $\chi \ne 0$  the coefficient of chemicatic sensitivity; a > 0 the natural growth rate of cellular population; and K > 0 the typical carrying capacity of cellular population. Equation (1) depicts the movement of a cellular population in response to a chemical signal (chemotaxis), while both entities are naturally diffusing, growing/dying and producing/degrading in the local environment.

Under the assumption  $\chi \mu > 0$ , via the inverse Hopf-Cole transformation  $v = (\ln s)_x$  and rescaling, (1) is converted into a system of hyperbolic-parabolic balance laws:

$$\begin{cases} v_t + (u - \varepsilon v^2 / \chi)_x = \varepsilon v_{xx}, \\ u_t + (uv)_x = Du_{xx} + ru(1 - u), \end{cases}$$
(2)

where  $\varepsilon \ge 0$ , D > 0, and  $r = aD/(\chi \mu K) > 0$ . We study Cauchy problem of (2):

$$v(x,0) = v_0(x), \quad u(x,0) = u_0(x), \qquad x \in \mathbb{R},$$
(3)

where  $(v_0, u_0)$  is a perturbation of the constant equilibrium state (0, 1).

In this talk we survey a sequence of recent results for (2), (3) on global existence and large time behavior [1-7]. In particular, we focus on the optimal  $L^2$  time decay rates for large data solutions and detailed, pointwise convergence of small data solutions to explicitly constructed asymptotic solutions, corresponding to different scenarios of the chemical concentration *s*.

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#### **Application of Fractional Calculus to Image Denoising**

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Removal of noise is an important step and a challenging problem in the image processing. Denoising is a process used to remove the noise from the corrupted image, while retaining the edges and other detailed features as much as possible. Recently, denoising in the fractional domain is a hot research topic [1, 2]. The fractional-order anisotropic diffusion method can cause less blocky effect and preserve edges in image denoising, which received much interests in literature. Based on this method, we propose a new method using fractional calculus to image denoising, which is different from the well-known method and called as fractional-varying-order differential method. We use it rather than constant-order differential in processing. We consider the following functional defined in the space of continuous images over a support of  $\Omega$  This equation is associated with the following energy functional:

$$E(u) = \int_{\Omega} f(|D_{\mathbf{A}}u|) \mathrm{d}\Omega \tag{1}$$

where  $\mathbf{A} = \alpha(| \bigtriangledown u |)$  and  $\alpha(\cdot)$  is an increasing function and meet the condition

$$\alpha(x) \to \begin{cases} 1, & x \to 0\\ 2, & x \to \infty \end{cases}$$

 $D_{\mathbf{A}}$  denotes the fractional-varying-order differential operator defined by  $D_{\mathbf{A}}u = (D_{\mathbf{A}x}u, D_{\mathbf{A}y}u)$  and  $|D_{\mathbf{A}}u| = \sqrt{D_{\mathbf{A}x}^2 + D_{\mathbf{A}y}^2}$ .

The theoretical analysis and experimental results show that compared to state-of-the-art fractional-order anisotropic diffusion method(see Fig. 1), the proposed fractional-varying-order differential denoising model can preserve fine structure and texture well while quickly removing noise, and yield good visual effects and better peak signal to noise ratio.

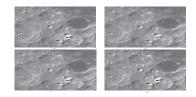


Figure 1: Denoising results of comparison of fractional-order anisotropic diffusion model and our proposed model on changeone. (a) Original image; (b) Damaged image with  $\sigma = 10$  Gaussian Noise (PSNR=24.1429); (c)fractional-order anisotropic diffusion model (PSNR=25.9132,  $\alpha = 1.2$ ); (d) Our proposed model (PSNR=26.2389).

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## Exponential stabilization for Markovian neural networks with additive time-varying delays via sample-based event-triggered impulsive control

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This paper investigates the Exponential Stabilization (ES) problem for Markov Jump Neural Networks (MJNNs) with Additive Time-varying Delays (ATDs). To mitigate the waste of networks or social resources, a new samplebased Event-triggered Impulsive Control Scheme (EICS) is proposed. Firstly, based on the Lyspunov theory, a novel Lyapunov-Krasovskii Functional (LKF) is constructed, which contains more information about ATDs and Markov jump parameters. Under the new EICS, by employing Wirtinger inequality and other analysis techniques, a less conservative ES criterion for the studying system is then presented in terms of Linear Matrix Inequalities (LMIs). In the end, a numerical example is given to illustrate the feasibility and validity of the obtained result.

MJNNs with TDs, as a special kind of hybrid systems, which have received much more attention in the past decades. However, the TDs generated among different nodes in practical NNs, named that ATDs, which may be distinct in their physical properties. From this point of view, it is not reasonable anymore if we regard the ATDs as the same one. Therefore, it is meaningful to study the control and synthesis for MJNNs with ATDs [1]:

$$\begin{cases} \dot{x}(t) = -B_{r_t}x(t) + A_{r_t}f(x(t)) + D_{r_t}f(x(t-d_1(t)-d_2(t))), \ t \in [t_k, t_{k+1}), \\ x(t_k) = (E+C_{r_t})x(t_k^-), \ x(t+\theta) = \varphi(\theta), \ \forall \theta \in \mathbb{I} = [-\max(d_1+d_2), 0]. \end{cases}$$
(1)

On the other hand, to mitigate the waste of networks or social resources, the EICS has been widely applied to various hybrid systems. Generally, the traditional EICS whose Triggered Function (TF) is described as

$$t_{k+1} = \inf\{t|t > t_k, \|x(t_k) - x(t)\| \ge \gamma \|x(t_k)\|\}.$$
(2)

However, it has some disadvantages [2]. In order to further save the cost of resources and overcome the shortages of the traditional EICS, a new sample-based EICS is proposed in this paper, i.e.  $t_{k+1} = t_k + l_m h$  with

$$l_m = \min\{l_1, l_2 | F_1(l_1) \ge 0, F_2(l_2) < 0\},\tag{3}$$

where  $F_1(l_1) = x^T(t_k + l_1h)\Omega_i x(t_k + l_1h) - (1 + \alpha_{r_t})x^T(t_k)\Omega_{r_t} x(t_k)$ ,  $F_2(l_2) = e^T(t_k + l_2h)\Omega_{r_t} e(t_k + l_2h) - \alpha_{r_t} x^T(t_k)\Omega_i x(t_k)$ ,  $e(t_k + l_2h) = x(t_k + l_2h) - x(t_k)$ , h is a constant sampling period,  $l_1 \in \mathbb{N}$  and  $l_2 \in (1, 2, 3, \dots, L] \subset \mathbb{N}$  and L is a relatively large integer number,  $\Omega_i$  are the weight matrices to be determined,  $\alpha_{r_t} \in (0, 1]$  are the triggered thresholds.

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## **Event-Triggered Control of Time-Delay Systems**

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Compared with the traditional approaches for updating the feedback control, the event-triggered control method is to update the control inputs when it is needed. The general research topic of event-triggered control of dynamical systems is to determine when the control signals need to be updated to improve efficiency while still guaranteeing the desired performance. The event-triggered control method has been widely investigated for various control problems recently. On the other hand, time-delay is ubiquitous in many practical systems since everything takes time to happen. Due to the advantage of event-triggered control in efficiency improvements and the significance of time-delay systems in modeling the real-world phenomena, it is crucially needed to study the event-triggered control of time-delay systems, which motivates this research.

There are two main challenges in this study. First, the control algorithms for delay-free systems cannot be applied to time-delay systems directly. Another challenge, which is also the main difficulty of this research, is to exclude the Zeno behavior from the proposed event-triggered control algorithms. In this talk, we will introduce an event-triggered control algorithm which is based on the Lyapunov-Razumikhin technique. However, Zeno behavior can be easily examined in linear time-delay systems. Therefore, a hybrid event-triggered control and impulsive control mechanism will be proposed to rule out the Zeno behavior.

## A Weak iISS Notion for Impulsive Systems with Time-Delay

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The impulsive system is a hybrid dynamical system that exhibits both continuous dynamics (modeled by differential equations) and discrete dynamics (or impulses which are state jumps or resets at a sequence of discrete moments). Due to the ubiquitous of time-delay, the stability of impulsive time-delay systems has been studied extensively in the literature (see, e.g., [1, 2]). The notion of input-to-state stability (ISS), introduced by Sontag in [3], characterizes the impact of external inputs to the control system. The ISS notion roughly states that "the state must be bounded if the external inputs are uniformly bounded". However, the boundedness of the states cannot be reflected through the ISS property when the inputs are unbounded but have finite total energy (e.g., impulse inputs). Another drawback of the ISS property is that it cannot provide an ideal bound if the external inputs have an extremely large bound but finite total energy. To take into account of such inputs, an integral variant of ISS, called integral input-to-state stability (iISS), was introduced in [4].

In this talk, we will introduce a new iISS notion for impulsive systems with time-delay which is weaker than the widely used one initialed in [4] and more applicable to systems with delay-dependent impulses. We study the integral input-to-state stability of nonlinear time-delay systems with delay-dependent impulses. The stability analysis is conducted by using the method of Lyapunov-Krasovskii functionals. In general, the Lyapunov candidate is broken into a function part and a functional part in order to follow the spirit of Lyapunov and Krasovskii and characterize the impulse effects simultaneously. To be more specific, the instantaneous state jumps can be captured through the function part of the Lyapunov candidate, while the functional part is indifferent to impulses. The main contribution of this research is that the iISS results are derived for impulsive systems with time-delay in both the continuous dynamics and the impulses. Additionally, compared with the results in [5, 6], our iISS criteria are less conservative when applied to time-delay systems with delay-free impulses.

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## A Hierarchical Neural Model for Sequential Data Classification

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Accurate text classification is a key task in many applications, such as sentiment analysis, topic labeling, spam detection, intent detection and Information Retrieval. In this work, we particularly focus on the classification for a sequence of textual data, for example, the user behaviors at a site, with the aware of the dynamic characteristic of the intent. Previous approach in text classification include conventional classification approaches such as Naive Bayes classifier, Gradient Boosting Trees, Support Vector Machine, Random Forest with manually crafted features [3], sequential learning model, such as Conditional Random Field (CRF) [1]. In recent years, the popular neural models are emerging in various applications. Convolutional Neural Networks (CNN) has been adopted to extract vector representations as the features for Random Forest to classification, the deep model has obtained higher performance compared to conventional classification approaches and variations of CNN models in [4]. The Global Vectors model enriched word embedding vectors with multiple Bidirectional LSTM layers is proposed in [5] to understand textual intent.

In this work, our sequential data is obtained from an E-commerce site, and the goal is to detect the meaning of the query within a search session. The query classification is not a trivial task, and we summarize the main challenges in finding the best matching categories for a sequence of queries as follows. (1) Unbalanced Categories: Some categories are more popular than the other, and the popular categories could expose tens of thousands of more times than the unpopular categories. (2) Dynamic Intents: The intent of the same text may not be the same with different customers, or even with the same customer under different circumstances. For instance, "Apple" could mean a brand with several categories of electronic products, or a type of fruit. (3) Lack of Annotated Data: It is very labor extensive to manually label large amount of data for a deep neural model to train. Inspired by the above challenges, we design a hierarchical deep learning framework which learns the multi-directional interdependencies within a point in the sequence, as well as the forward dependencies among the points of the sequence. The proposed framework has three major modules. We first build a query-based module, which has a bidirectional (forward and backward) Recurrent Neural Networks (RNN) with Gated Recurrent Unit (GRU) to learn the encoding of the words in the query. Then an attention mechanism generates dynamic query representations from the word encoders. The second module is at the session level, which uses self attention and GRU dropout techniques to learn the dependencies between the queries and to avoid overfitting. The last step takes the session annotations and the query annotations as inputs and classifies the data.

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## Effects of Charge Noise on a Spin Qubit in Silicon

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Research on physical implementation of quantum computing has made dramatic progress over the past decade, spearheaded by superconducting qubits and trapped ion qubits, to the degree that small-scale quantum information processors should be within reach over the next few years. Studies of semiconductor spin qubits, which have often been considered one of the most promising in terms of scalability, have also yielded some important results in the past decade in demonstrating exceptional coherence properties for single spins confined in quantum dots and donors and high-fidelity single-qubit gates. Spin qubits, however, still suffer from low fidelity in two-qubit gates, making any computation involving multiple gates (such as quantum error correction) impossible.

In this talk I will discuss how charge noise can affect spin qubits via spin-orbit interaction or inhomogeneous magnetic field produced by a micromagnet. We derive a non-Markovian Master equation for a spin qubit and identify memory effects due to the nonlocal noise correlation. We then apply this Master equation in the specific case of a single electron in a double quantum dot that is under the influence of a micromagnet, and demonstrate how charge noise leads to both spin relaxation and spin dephasing.

We thank financial support by US ARO.

## **Convolutional Neural Network with Attention-based Layer for Text Classification**

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Text classification is the most critical basis for Information Retrieval(IR) [1]. In the past, text classification tasks are highly dependent on feature engineering. N-Gram, and weighted words, such as Term-Frequency(TF) and Term Frequency-Inverse Document Frequency(TF-IDF), are commonly used text features [2, 3, 6]. However, feature extraction usually is time-consuming and complex, especially when the size of the vocabulary in the corpus reaches millions, feature extraction approaches face computational challenges that are difficult to solve. More important, these features suffer from distinct limitations. Words are treated as individual atoms by these features, the similarity between words and semantics meanings are neglected. Neural network models have achieved stateof-the-art performances in a wide range of domains, including various IR applications. As a classic deep neural network architecture, Convolutional Neural Networks(CNNs) have the ability to automatically extract features from unstructured data. Therefore, in this paper, a document-level classification model based on convolutional neural network with attention mechanism layer is proposed. The model contains a word representation layer, convolutional layers and attention mechanism layer. For acquiring machine understandable input, word embedding is employed to project the bag-of-words into N-dimensional vector spaces [5]. Different from the traditional CNNbased classifier, a attention mechanism layer is deployed after the convolutional layer extracting the representations from the word vectors. The attention layer enhances the significance of key features and focused word by assigning attention weights from different context windows [4]. The output layer of the classifier is a softmax function, which is fully connected with the feature vector. The experiment is conducted on the THUCNews dataset, which is collected from the historical data Sina News RSS subscription channel from the year of 2005 to 2011, containing 740,000 Chinese News articles with 14 candidate categories. The percision, recall, and F1-score are investigated as the evaluation measurements. The result demonstrates that good performance has achieved in terms of the classification accuracy.

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## **Uncertainty in Machine Learning for Energy Forecasting**

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Estimating the future electric load is key to decision making and planning for electric utilities. Recent work has shown the efficacy of machine learning techniques such as long short-term memory neural networks and gradient tree boosting in forecasting time series data for a variety of applications. However, such predictions do not come with a confidence estimate, which can be dangerous when mission critical decisions are being made. We propose and demonstrate two methods for evaluating the uncertainty in electric load predictions, using Monte Carlo dropout on an LSTM neural network model to perform Bayesian deep learning and quantile regression on a gradient boosting model. We train neural network and gradient boosting regressor models on real-world electric load data and show that an uncertainty estimate can be obtained alongside the predictions with minimal drop in accuracy.

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## Predictive temperature-driven multi-year modeling and risk assessment of West Nile virus in southern Ontario, Canada

#### ABSTRACT:

We develop a temperature-driven multi-year transmission model for West Nile virus (WNV) vector species, Culex pipiens and Culex restuans. The model explicitly considers the impact of daily temperature on mosquito biology and disease transmission between mosquitoes and birds. Employing the use of a linear degree day function to track the progression of the virus through the extrinsic incubation period (EIP) enabled the model to capture the general trend and appearance of the disease observed in mosquito surveillance data. Analysis of numerical results highlight an important relationship between adult female mosquito longevity and the EIP—both of which are influenced by temperature. Using observed and forecasted mean daily temperatures we demonstrate the capacity of the model to be used as a predictive risk assessment tool to inform public policy in the fight against WNV outbreaks.

## A 3D IB Method for non-Newtonian-Fluid Flexible-Structure Interaction

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Fluid-flexible-structure-interaction (FFSI) is complex and challenging to model and simulate, and it is still an area of active research. Motivated by FFSI phenomena in life sciences (e.g., motions of red blood cells and cytoskeleton in complex fluids), we introduce a new immersed boundary method for FFSI problems involving non-Newtonian fluids in three dimensions. The non-Newtonian fluids are described by the FENE-P model. The fluid flow is modelled by the lattice Boltzmann equations (the D3Q19 model). The deformable structure and the fluid-structure-interaction are treated by the immersed boundary method [1]. As a test for the new method, four toy FFSI problems are considered --- an elastic flexible sheet being towed at its midline or being rotated at one edge constantly and the sheet being flapped sinusoidally at its leading edge or at its midline periodically. In all the cases the structure is immersed in a stationary FENE-P fluid in a three-dimensional periodic domain [2-3].

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## Equilibria of the Curved N-body Problem in S<sup>n</sup>

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While equilibrium does not exist in the Newtonian N-body problem, they do exist in the curved N-body problem in  $S^3$ . We will construct examples of them. We then extend the study of equilibrium to  $S^n$  and discuss one class of equilibria in  $S^n$ , the Dziobek equilibria, that are formed by n+2 bodies on  $S^n$ . This is an analogy of Dziobek central configurations of the Newtonian N-body problem. We obtain a criterion for them and reduce it to two sets of equations.

#### **Characterizing Pulse Waves for Disease Diagnosis**

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Pulse waves contain a wealth of human physiological and pathological information. Over 2000 years, traditional Chinese medical (TCM) doctors have used pulse wave information for disease diagnosis and treatment assessment. However, lack of quantitative standardization and mathematical explanation makes TCM less acceptable in western medicine [1]. Therefore, the quantification and standardization of TCM pulse diagnosis must be addressed.

In this paper, we aim to characterize digitalized pulse waves associated with healthy and diseased pulse waves. First, we collected digitalized pulse data of healthy and diseased subjects, acquired by the pulse diagnosis instrument designed by The King's Pulse Science and Technology Company Limited [2]. The data was sampled at 400 Hz. Then we examine pulse waves in temporal, frequency or joint temporal-frequency domain [1, 3, 4].

Our results suggest that the clinically relevant characteristics of pulse waves can be revealed in time, frequency and time-frequency domain using different transforms. Quantitative measures that reflect the peak width, ratio of peak heights and curvatures of pulse waves can be developed by combining and extracting these characteristics in all three domains. This work aims to lay the ground work for our future work on pulse wave information extraction and classification for clinical purposes.

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## **Creation of a Model for Efficient Management of a Sustainable Development of a Region as an Organizational System**

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For an organizational system to be successful availability of complete information and leveraging intellectual resources is a must. In any situation subjects make decisions relaying on the informational processes, through which the subjects and objects interact.

For efficient operation of the organizational systems we have to develop alternative scenarios of its operation.

The publication deals with the issues of the organizational management in terms of sustainable development of regions for their efficient management determines the sustainable development of a country.

In order to study the problems concerning the regional management we have to investigate to what extent the regional development factors (indicators) influents its characteristic criteria. Such criteria are numerous indeed and so are the scenarios to be investigated [1,2,3]

In the publication we discussed:

- selection of subspace of highly important (highly influential) basic factors out of space of the regional development factors
- creation of an organizational management model on the grounds of the derived factors

In the study we employ the methods of cognitive modeling, statistical analysis, the theory of implicit multitude and diagrams.

The results will be presented on both the fundamental and applied level.

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# Direct measure of genuine tripartite entanglement independent from bipartite constructions

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A measure of non-Gaussian entanglement in continuous variable (CV) systems based on the volume of the negative part of the Wigner function is proposed. We analyze comparatively this quantity with a numerical evaluation of the negativity of partial transpose (NPT) considering a system of Bell states formed in the coherent state basis (quasi-Bell states).

## A Novel Quantum Algorithm Based Entanglement measure to classify incomplete patterns

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Following [1], in this paper, we develop a novel classification algorithm that is based concurrence as of entanglement measures to classify incomplete patterns. The proposed algorithm classifies an input into one of two binary classes even if the input pattern is incomplete. The proposed algorithm applying unitary operators to conduct the competition between neurons in order to find the winning class based on wining-take-all. Then, we derive a formula from concurrence, C, relation [1] as follows

$$C = 2\frac{\sqrt{m0(N-m0)}}{N},\tag{1}$$

to find the most closest patterns to the input pattern. The novelty of the proposed algorithm is shown in its application to the quantum computer. Our idea is validated via classifying the state of Reactor Coolant Pump of a Risky Nuclear Power Plant and compared with other quantum-based competitive neural networks model.

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## Fair Division of Graphs and of Tangled Cakes

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Recent work by Bilò et al [1] concerns allocating graph vertices (treated as indivisible objects) so that each share forms a connected subgraph, and so that no agent x envies another's share "up to one good" – any envy x has for y's share is erased if x pretends y did not receive her most valued vertex. Their methods are adapted from the cake-cutting literature, wherein the unit interval [0,1] serves as a model for the continuous "cake." But the discrete analogue of [0,1] is a path graph, so most of their results apply only to path graphs (and Hamiltonian graphs, which add edges to a path graph). For non-Hamiltonian graphs, the continuous analogue is more complicated than [0,1]; several copies of [0,1] are glued at their endpoints to form the letter Y, or the figure 8, or something more complex . . . a "tangle." We give some positive and negative results for envy free division of tangles, and discuss their implications for the original problem of graph division.

We look forward to welcoming you in Waterloo, Canada at the AMMCS-2019 Conference!

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#### Using supermodeling in computer simulation of complex systems

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We define the supermodel as a coupled ensemble of a few "imperfect" dynamic sub-models { $\mu$ , $\nu$ ...} each described by the state vector  $\mathbf{x} = (x_1,...,x_i,...,x_m)$  such that

$$\dot{x}^{i}_{\mu} = f^{i}_{\mu}(x_{\mu}, t) + \sum C^{i}_{\mu\nu}(x^{i}_{\nu} - x^{i}_{\mu}) \text{ and } x_{sumo}(C, t) \equiv \frac{1}{M} \sum x_{\mu}(C, t)$$
(1)

where the coefficients  $C_{\mu\nu}$  of matrix C are the coupling factors synchronizing the sub-models, and  $x_{sumo}$  is the supermodel output calculated as the ensemble average. Unlike the original application of supermodeling in climatology (Ref. [1]), used for increasing the climate forecast accuracy by tight coupling ( $\mathbf{C}$  is dense) of a few very complex heterogenous climate models (see Fig.1a), we propose to employ supermodeling in a much broader perspective. Herein we demonstrate that the loosely coupled supermodel (C is sparse) can be used as a second abstraction layer in data assimilation (DA) procedure. The standard DA algorithms, however, such as approximate Bayesian computations (ABC), suffer the curse of dimensionality problem. Consequently, the time complexity of ABC procedure grows exponentially with the number of parameters what make it useless for multiscale and/or sophisticated models such as 3D tumor model (Ref.[2]). Instead, we propose to create the supermodel which couples a few instances of the reference model (see Fig.1b). These sub-models can represent various local minima of the  $F(||\mathbf{x}-\mathbf{x}_{ground\_truth}||)$  cost function in the parameter space, found during initial phases of ABC data adaptation to the reference model. They are coupled only through the most sensitive dynamical variable (see Fig.1b). Next, the ABC procedure (or the other DA procedure presented in Ref.[1]) will be used for matching only a few coupling factors in the supermodel instead tens of parameters in the reference model. We discuss the advantages and problems we encountered in using this concept for DA both for toy dynamical systems and complex models, such as N-body, population and cancer dynamics. We conclude that the supermodeling is a very effective and generic procedure, not only as a method for increasing predictive accuracy of the computer models but also as an efficient computational framework for data assimilation.

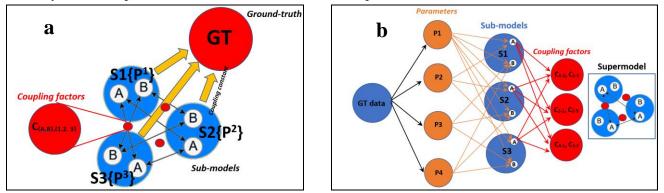


Figure 1: The supermodeling concept (a) and its application as a second abstraction layer in data assimilation. S1-S3 are the sub-models, P1-P4 model parameters, A and B dynamical variables and GT (ground truth) the real data.

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