CAIMS Annual Meeting 2021

Abstracts & Schedule

June 21-24, 2021

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Plenary Talks

Representation and Learning in Graph Neural Networks

Stefanie Jegelka

Electrical Engineering and Computer Science, Massachusetts Institute of Technology, USA

Graph Neural Networks (GNNs) have become a popular tool for learning representations of graph-structured inputs, with applications in computational chemistry, recommendation, pharmacy, reasoning, and many other areas.

In this talk, I will show recent results on representational power and learning in GNNs. First, we will address representational power and important limitations of popular message passing networks and of some recent extensions of these models. Second, we consider learning, and provide new generalization bounds for GNNs. Third, although many networks may be able to represent a task, some architectures learn it better than others. I will show results that connect the architectural structure and learning behavior, in and out of the training distribution.

This talk is based on joint work with Keyulu Xu, Jingling Li, Mozhi Zhang, Simon S. Du, Ken-ichi Kawarabayashi, Vikas Garg and Tommi Jaakkola.

Vaccination strategies for highly mutable pathogens: from statistical physics to monkeys

Arup Chakraborty

Department of Chemical Engineering, Department of Physics, Department of Chemistry, and Institute for Medical Engineering & Science, Massachusetts Institute of Technology, USA

Efforts to develop effective vaccines against highly mutable pathogens have largely been unsuccessful. HIV is a prominent example. We do not have a universal vaccine that can protect us from diverse strains of influenza either. I will describe how bringing together theory/computation (rooted in learning algorithms and statistical physics) with basic and clinical immunology can help address such challenges. Using such an approach, we translated data on HIV protein sequences to knowledge of the HIV fitness landscape ? i.e., how the virus? ability to propagate infection depends on its sequence. Predictions emerging from the fitness landscape were then tested against in vitro and clinical data. I will discuss how a potentially potent T cell-based therapeutic vaccine was designed based on these findings and tested positively for immunogenicity in rhesus macaques. If time permits, I will also describe work aimed toward eliciting antibodies that can protect against diverse strains of highly mutable pathogens. This is a problem at the intersection of statistical physics, immunology, and learning theory.

The seven-league scheme: deep learning for large time step Monte Carlo simulation of SDEs

Kees Oosterlee

Mathematical Institute, Utrecht University, the Netherlands

We propose an accurate data-driven numerical scheme to solve Stochastic Differential Equations (SDEs), on the basis on using large time steps. The SDE discretization is based on a polynomial chaos expansion method, and accurately determined stochastic collocation (SC) points. By an artificial neural network these SC points are learned. We then perform Monte Carlo simulations with large time steps. Error analysis confirms that this data-driven scheme results in accurate SDE solutions in the sense of strong convergence, provided the learning methodology is robust and accurate. With a variant method called the compression-decompression collocation and interpolation technique (CDC), we reduce the number of neural network functions that have to be learned, so that computational speed is enhanced. Numerical results show high quality strong convergence error results, when using large time steps, and the novel scheme outperforms some classical numerical SDE discretizations. Some applications, in financial option valuation, are presented.

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TBA

Hansi Alice Singh

School of Earth and Ocean Sciences, University of Victoria, Canada

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Graphon Mean Field Games: A Dynamical Equilibrium Theory for Large Populations on Complex Networks

Peter Caines

Department of Electrical and Computer Engineering, McGill University, Canada

The complexity of large population multi-agent dynamical systems, such as occur in economics, communication systems, and environmental and transportation systems, makes centralized control infeasible and classical game theoretic solutions intractable.

In this talk we first present the Mean Field Game (MFG) theory of large population systems. Going to the infinite population limit, individual agent feedback strategies exist which yield Nash equilibria. These are given by the MFG equations consisting of (i) a McKean-Vlasov-Hamilton-Jacobi-Bellman equation generating the Nash values and the best response control actions, and (ii) a McKean-Vlasov-Fokker-Planck?Kolmogorov equation for the probability distribution of the states of the population, otherwise known as the mean field. The applications of MFG theory now extend from economics and finance to epidemiology and physics.

Next we introduce Graphon Mean Field Game and Control theory. Very large scale networks linking dynamical agents are now ubiquitous, with examples being given by electrical power grids and social media networks. In this setting, the emergence of the graphon theory of infinite networks has enabled the formulation of the Graphon Mean Field Game equations, and, in recent work, we have established conditions for the existence and uniqueness of solutions to the GMFG equations. As in the special case of MFG theory, it is the simplicity of the infinite population GMFG strategies which permits, in principle, their application to otherwise intractable problems involving large populations on large complex networks.

Tackling the curse: polynomial and deep neural network methods for function approximation in high dimensions

Ben Adcock

Department of Mathematics, Simon Fraser University, Canada

Many problems in computational science and engineering require the accurate approximation of a target function from data. This problem is rendered challenging by the high-dimensionality of the function, the expense of generating function samples, the presence of noise in the measurements, and the fact that the target function may take values in a function space. Developing techniques that tackle these challenges without succumbing to the famous "curse of dimensionality" has been a long-standing problem.

In the first part of this talk I will give a brief survey of a decade?s worth of progress on high-dimensional function approximation via sparse polynomial expansions. I will show how the proper use of compressed sensing tools leads to algorithms for high-dimensional approximation which, unlike other approaches, possess provably near-optimal error bounds and moderate sample complexities. In particular, these techniques mitigate the curse of dimensionality to a substantial degree. The second part of the talk will be devoted to emerging approaches based on deep neural networks and deep learning. Such tools are beginning to garner substantial attention in the scientific computing community. Nonetheless, I will present evidence of a key gap between current theory and practice. I will then discuss recent results showing that there exist deep neural networks that match the performance of best-in-class schemes, and furthermore, these can indeed be trained through realizable procedures. This highlights the potential of deep neural networks, and sheds light on achieving robust, reliable and overall improved practical performance.

This talk is based on joint work with Anyi Bao, Simone Brugiapaglia, Juan M. Cardenas, Nick Dexter, Sebastian Moraga, Yi Sui and Clayton G. Webster.

Prize/Award Talks

The closest point method for solving partial differential equations on surfaces

Steve Ruuth

Department of Mathematics, Simon Fraser University, Canada

The numerical approximation of partial differential equations (PDEs) on surfaces poses interesting challenges not seen on flat spaces. The discretization of these PDEs typically proceeds by either parametrizing the surface, triangulating the surface, or embedding the surface in a higher dimensional flat space. Here we consider an embedding method, the closest point method, which is designed to solve a variety of PDEs on smooth surfaces using a closest point representation of the surface and standard Cartesian grid methods in the embedding space. An attractive property of the method, in its explicit form, is that it frequently leads to evolution equations that are simply the equations of the corresponding flow in the embedding space. This advantage means that with the insertion of a simple interpolation step, highly effective 3D numerical PDE codes can be reused to approximate the evolution of PDEs on surfaces. In this talk, we review the closest point method and present recent results for solving PDEs on moving surfaces, as well as recent domain decomposition methods and software suitable for parallel computing.

Formal Methods for Control of Dynamical Systems

Jun Liu

Department of Applied Mathematics, University of Waterloo, Canada

Motivated by safety-critical control of cyber-physical engineering systems, formal methods for control aims to synthesize controllers for continuous dynamical systems to meet high-level specifications. Finite abstractions, also known as symbolic models, have provided useful means for algorithmically synthesizing hybrid controllers with respect to rigorous specifications (e.g., safety, reachability, or more generally a temporal logic formula). A central theoretical question surrounding abstraction-based control is whether one can decide, through finite abstractions and discrete synthesis, the existence of a controller for a nonlinear system to satisfy a given specification. This question may also have practical implications towards addressing the inherent scalability issues of abstraction-based approaches.

In this talk, we discuss some recent results towards answering this question. We first introduce a method to synthesize robust controllers for temporal logic formulas using finite abstractions. We then use this notion of robustness to show that, if a system robustly satisfies a given specification, then it is possible to use discrete abstractions to synthesize a robust controller. Following this, we present a specification-guided framework to improve the computational performance of abstraction-based methods, while providing the same theoretical guarantees. We conclude by arguing that the intrinsic robustness and controllability of the underlying dynamical system can and should be exploited to address the scalability issues caused by discretization of continuous dynamics and to mitigate the combinatorial explosion imposed by logic specifications.

Our muscles aren't one-dimensional fibres

Nilima Nigam

Department of Mathematics, Simon Fraser University, Canada

Skeletal muscles possess rather amazing mechanical properties. They are comprised of several tissues, possess an intricate structure, and behave nonlinearly in response to mechanical stresses. In the 1910s, A.V. Hill observed muscles heat when they contract, but not when they relax. Based on experiments on frogs he posited a mathematical description of skeletal muscles which approximated muscle as a 1-dimensional nonlinear and massless spring. This has been a remarkably successful model, and remains in wide use. Yet skeletal muscle is three dimensional, has mass, and a fairly complicated structure. Are these features important? What insights are gained if we include some of this complexity in our models? Complex models can suffer from 'over-fitting' of parameters - how can this be addressed? In this talk, we'll see (partial) answers to some of these questions.

This work was done as part of a long-standing collaboration with James Wakeling's lab at SFU.

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Infectious Disease Dynamics from the Black Death to COVID-19

David Earn

Department of Mathematics and Statistics, McMaster University, Canada

Historical records allow us to reconstruct patterns of disease spread in the past, in some cases going back hundreds of years. Mathematical models can help us reveal the mechanisms that shaped these epidemics. I will discuss analyses that identify how demographic and behavioural processes changed the structure of recurrent epidemics of childhood infections, such as measles and whooping cough, in the 20th century. I will also describe recent work that illuminates epidemic patterns as far back as the Black Death in the 14th century, and how COVID-19 presents some of the same, and some very different, challenges.

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Multi-marginal optimal transport: the good, the bad and the ugly

Brendan Pass

Department of Mathematical and Statistical Sciences, University of Alberta, Canada

Optimal transport is the general problem of trying to pair two distributions of mass (the marginals) with maximal efficiency, relative to a given cost function (think, for example, of using a pile of dirt to fill a hole of the same volume, so as to minimize the average distance the dirt moves). This is a vibrant area of modern mathematics, touching on analysis, partial differential equations, geometry and probability, with far reaching and diverse applications in areas such as meteorology, operations research, fluid mechanics, finance and biology, to name only a few. Solutions to this problem are by now fairly well understood; in particular, under reasonable conditions, they concentrate on graphs over the first variable.

Over the past decade, largely driven by its own diverse collection of applications (including, for example, matching agents in multi-sided markets in economics, interpolating among distributions in data science, and minimizing interaction energies between electrons in quantum physics) interest has grown rapidly in multi-marginal optimal transport, in which there are several, rather than two, distributions to be matched. Solutions to this problem exhibit an intricate dependence on the cost function. For some costs, solutions concentrate on graphs over the first variable as in the more classical, two marginal case (I think of this

structure as "good"), whereas for others, solutions can be much more exotic (I think of this structure as "bad," or in the worst cases, "ugly"). In this talk, I will survey the state of the art, and in particular attempt to develop some intuition for the dichotomy between these two types of costs, illustrating the discussion with examples arising in physics, economics, and data science. If time permits, I will briefly discuss some ongoing work and point to some open problems.

Invited Theme Sessions

Mathematical Biology 1

Organizer: **Sue Ann Campbell, Mohammad Kohandel**

Establishing improved combination therapies in oncology using quantitative medicine

Morgan Craig

Département de mathématiques et de statistique, Université de Montréal, Canada

Despite the long-term concerted investment in highly-intensive cancer research, the goal of precision and personalized medicine remains largely out of reach. Establishing new cancer treatment strategies is difficult, as evidenced by the low regulatory approval rates of new drugs in oncology. Even with the approval of effective immunotherapies against certain cancers, including oncolytic viruses and immune checkpoint inhibitors, many immunotherapies have failed in trials. New approaches propose combining immunotherapeutic strategies to bolster efficacy, but how to optimally design combination treatments and select the patient populations in which they will be effective remains a challenge. Given these many complexities, solutions are needed for new approaches to preclinical drug development in oncology. In this talk, I will discuss our efforts to rationalize the drug development process of novel combination therapies against cancer by merging in vitro, in vivo, and in silico models using quantitative medicine.

A systems biology approach to decode how cancer cells switch among different phenotypes during metastasis and therapy resistance

Mohit Kumar Jolly

Centre for BioSystems Science and Engineering, Indian Institute of Science, India

Metastasis (the spread of cancer cells from one organ to another) and therapy resistance cause above 90% of all cancer-related deaths. Despite extensive ongoing efforts in cancer genomics, no unique genetic or mutational signature has emerged for metastasis. However, a hallmark that has been observed in metastasis is adaptability or phenotypic plasticity – the ability of a cell to reversibly switch among different phenotypes in response to various internal or external stimuli. Phenotypic plasticity has also been recently implicated in enabling the emergence of resistance for many cancers across multiple therapies. However, a mechanistic understanding of these processes from a dynamical systems perspective remains incomplete.

This talk will describe how mechanism-based mathematical models for phenotypic plasticity can enable our improved understanding of cellular decision-making for multiple perspectives: a) Multistability (how many cell states exist en route?) b) Reversibility/irreversibility (do cells come across a ?tipping point? at specific time and/or dose of inducers beyond which they do not revert?) c) Hysteresis (do transitioning cells

follow same/different paths?) d) Design principles of networks (are there topological signatures in networks enabling phenotypic plasticity that can be exploited for therapeutic purposes?)

Collectively, our work highlights how an iterative crosstalk between mathematical modeling and experiments can both generate novel insights into the emergent nonlinear dynamics of cellular transitions and uncover previously unknown accelerators of metastasis and therapy resistance.

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One size doesn't fit all: optimizing cancer immunotherapy

Jana Gevertz

Department of Mathematics & Statistics, The College of New Jersey, USA

Mathematical models of biological systems are often validated by fitting to the average behavior in an often small experimental dataset. Here we ask the question of whether mathematical predictions for the average are actually applicable in samples that deviate from the average. We will explore this in the context of a mouse model of melanoma treated with two forms of immunotherapy: immune-modulating oncolytic viruses and dendritic cell injections. We will demonstrate how a mathematically optimal protocol for treating the average mouse can lack robustness, meaning the ?best treatment for the average? can fail to be optimal (and in fact, can be far from optimal) in mice that differ from the average. We also show how mathematics can be used to identify an optimal treatment protocol that is robust to perturbations from the average. We end by comparing the results of our robustness analysis to the personalized optimal protocol for each mouse in our experimental dataset.

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Capturing Individual Heterogeneity in a Deterministic Model of Cancer Immunotherapy: The 'Standing Variations Model'

Harsh Jain

Department Mathematics & Statistics University of Minnesota Duluth, USA

Studying rare outcomes in human diseases such as cancer is challenging because observation of the rare event may require a very high number of patients or experimental animals. In this talk, I will present our new, predictive approach – Standing Variations Modeling – to understanding the mechanisms underlying such rare events. I take as a case-study, the treatment of metastatic, castration-resistant prostate cancer with one of the the first FDA-approved live cell anti-cancer vaccines, sipuleucel-t (Provenge). However, its survival benefit remains modest, and an optimal dosing schedule has not been established, even after a decade of use. That is, the clinical success of sipuleucel-T is a rare event. Here, I will present our mechanistic model of prostate cancer growth and response to immunotherapy, that is calibrated with data from mouse xenograft experiments. I will then introduce our modeling paradigm, which captures the inherent heterogeneity that characterizes individuals in a population, and provides an explanation for the observed clinical outcomes of treatment with sipuleucel-t. We also predict an optimal therapeutic regime that maximizes predicted efficacy of the vaccine for a small subset of a heterogeneous population. Our approach readily generalizes to a range of emerging cancer immunotherapies, and more generally, to predicting and understanding how a population responds to any intervention targeting a human disease.

Mathematical Biology 2

Organizer: **Sue Ann Campbell, Mohammad Kohandel**

Can we infer gene regulation dynamics from static snapshots of gene expression variability?

Andreas Hilfinger[a,b,c], Euan Joly-Smith[a], Jerry Wang[d]

[a]Department of Chemical & Physical Sciences, University of Toronto Mississauga

[b]Department of Mathematics, University of Toronto

[c]Department of Cell & Systems Biology, University of Toronto

[d]Division of Biology and Biological Engineering, California Institute of Technology, USA

Inferring functional relationships within complex networks from static snapshots of co-varying variables is a ubiquitous problem in science. For example, a key challenge of systems biology is to translate cellular heterogeneity data obtained from single-cell sequencing or flow-cytometry experiments into regulatory dynamics. I will show how static population snapshots of co-variability can be exploited to infer properties of gene expression dynamics when gene expression reporters probe their upstream dynamics on separate time-scales. This can be experimentally exploited in dual-reporter experiments with fluorescent proteins of unequal maturation times, thus turning an experimental bug into an analysis feature. I will present correlation conditions that detect the presence of closed-loop feedback regulation in gene regulatory networks. Furthermore, I will show how genes with cell-cycle dependent transcription rates can be identified from the variability of co-regulated fluorescent proteins. Similar correlation constraints might prove useful in other areas of science in which static correlation snapshots are used to infer causal connections between dynamically interacting components.

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Long-term protein-based memory through prion inheritance in single cells

Laurent Potvin-Trottier

Department of Biology, Concordia University, Canada

Information transfer from generation to generation using DNA is a fundamental property of biological systems. Various epigenetics mechanisms enable transient transfer of information in progenies. In this talk, we will discuss protein-based elements of inheritance through self-propagating, non-pathogenic prion domains. These prion domains are commonly found in yeast but have also recently been found in bacteria and higher eukaryotes, and by acting as a bistable switch, can propagate a functionally distinct cellular state. How this state is propagated through the population, and how it is stochastically lost, remains unknown. In this talk, we address these questions using the bacterial prion domain SSB from Campylobacter hominis, and by following thousands of single cells for dozens of cell divisions using a microfluidic device and quantitative time-lapse microscopy. We show that the prion state is propagated through two different mechanisms with distinct loss distribution functions, creating a highly heterogenous structure in the population. In our model system, stochastic loss of the prion state is driven by partitioning errors at cell division, with large aggregates being inherited by one of the two daughter cells. A stochastic model of the chemical reaction kinetics is built to recapitulate the properties of the system. Finally, we show that propagation of the prion state imposes a minimal burden on the cell yet appears to provide protective effects again stress conditions. Therefore, prion domains could provide a mechanism to create phenotypic heterogeneity in the population, by creating a small population of resistant cells.

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Challenges in modeling the transition period of childhood diseases from the pre-vaccine to vaccine era

Felicia Magpantay

Department of Mathematics and Statistics, Queen's University, Canada

Mathematical models of childhood diseases often employ homogeneous time-dependent transmission rates. These models can provide good agreement with data in the absence of significant changes in population demography or levels of transmission, such as in the case of pre-vaccine era measles in industrialized countries. However, accurate modeling and forecasting of transient dynamics after the start of mass vaccination has proved more challenging. This is true even in the case of measles which has a well understood natural history and a very effective vaccine. Here, we demonstrate how the dynamics of homogeneous and age-structured models can be similar in the absence of vaccination, but diverge after vaccine roll-out. We also propose methods to fit such models to long term epidemiological data with imperfect covariate information.

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A Model of COVID-19 Vaccination and Waning Immunity in Canada

Jane Heffernan

Department of Mathematics and Statistics, York University, Canada

We have developed an age- and immunity-structured model of COVID-19 infection and vaccination. The model assumes rates of waning immunity from infection and vaccination. It also includes different non-pharmaceutical interventions, including work-from-home, school closure, social distancing and mask wearing. In this talk I will discuss different outcomes of a Canadian-informed COVID-19 vaccination program given different types of vaccines and rollout strategies. I will also discuss scenarios for relaxation and mitigation strategies needed to inhibit a Fall 2021 resurgence.

Dynamical System/Control Theory 1

Organizer: **Kirsten Morris, Jun Liu, Amenda Chow**

Linear Distributed Parameter Systems (DPS) Moving Horizon Estimation Design

Stevan Dubljevic

Department of Chemical and Materials Engineering, University of Alberta, Canada

Well-known finite-dimensional moving horizon estimation theory of constrained optimal output estimation is extended to linear infinite-dimensional systems modelled by partial differential equations. The unbounded operators due to the point and/or boundary sensing are transformed into a discrete-time infinite-dimensional model with bounded operators using Cayley-Tustin transformation that ensures model equivalence among continuous and discrete time settings. The moving horizon estimator design utilizes the discrete time model and Riccati equation and accounts for estimation efficiency and physical constraints in input, disturbance and output in an explicit manner. The resulting moving horizon estimator design is formulated as a finite-dimensional constrained quadratic optimization problem solvable by standard optimization techniques and simulation examples are presented.

Approximations of Lyapunov functionals and input-to-state stability of nonlinear parabolic PDEs

Guchuan Zhu

Department of Electrical Engineering, Polytechnique Montr'eal, Canada

In general, it is challenging to apply the Lyapunov method to establish the ISS in Lp-norm for nonlinear PDEs with boundary or in-domain disturbances when $p \in [1, 2)$ due to the lack of appropriate Lyapunov candidates. In this talk, we will show how to construct approximations of Lyapunov functionals via a convex function, which may be an alternative for ISS analysis of nonlinear PDEs. Based on the approximations of Lyapunov functionals, we can prove, using the Lyapunov argument, the ISS in the spatial L1-norm or weighted L1-norm for a class of n-dimensional nonlinear parabolic PDEs with Robin/Neumann or Dirichlet boundary disturbances. In addition, we will also show the extension of the proposed method to the establishment of the ISS in the spatial Lp-norm and W1,p-norm for 1-D nonlinear parabolic PDEs with in-domain disturbances when $p \in [1, 2)$.

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Quadratic ODE and PDE models of drug release kinetics from biodegradable polymers

Michel Delfour

Department of Mathematics and Statistics, Université de Montréal, Canada

In order to achieve prescribed drug release kinetics over long therapeutic periods, bi-phasic and possibly multi-phasic releases from blends of biodegradable polymers are currently envisioned. The modelling of drug release in the presence of degradation of the polymer matrix and surface erosion is quite complex. Yet, simple reliable mathematical models validated against experimental data are now available to classify neat polymers and to predict the release dynamics from polymer blends. We survey a two-parameter quadratic ODE model that has been validated against experimental data for the release of paclitaxel from a broad range of biodegradable polymers and a quadratic semi-permeable membrane PDE model that mimics the ODE model and readily extends to curved complex geometries of drug eluding stents.

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Optimal control of the Richards' equation and optimal irrigation planning

Robert Guglielmi

Department of Applied Mathematics, University of Waterloo, Canada

Optimal irrigation planning requires to properly model the diffusion, percolation and infiltration of water in the soil. For this purpose, the Richards' equation has proven particularly effective to describe water flows with different types of uptake and hydraulic functions, accounting for different crops or types of soil. In this talk we propose an optimal control framework to optimize the water consumption while ensuring an efficient irrigation. This approach results in a boundary control of the Richards' equation and in an objective functional that maximizes the root uptake. Numerical simulations are provided to support the theoretical findings.

Dynamical System/Control Theory 2

Organizer: **Kirsten Morris, Jun Liu, Amenda Chow**

FaSTrack and LR-CAM: two novel applications of pursuit-evasion games

Mo Chen

School of Computing Science, Simon Fraser University, Canada

In this talk, we explore two recent applications of Hamilton-Jacobi-Isaacs solutions to pursuit-evasion games. We begin with FaSTrack, which solves the problem of Fast and Safe planning and Tracking by considering a pursuit-evasion game between two dynamic models of an autonomous system. We then discuss LR-CAM, a least-restrictive collision avoidance module, obtained from a combination of two-agent pursuit-evasion game solutions and reinforcement learning, to prevent collisions in multi-agent systems.

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Learning Nash Equilibria with Bandit Feedback

Maryam Kamgarpour

Department of Electrical and Computer Engineering, University of British Columbia, Canada

Decision-making in multi-agent systems arises in engineering applications ranging from electricity markets to communication and transportation networks. I discuss decision-making of multiple players with coupled objectives. In this setting, a Nash equilibrium is a stable solution concept, since no agent finds it profitable to unilaterally deviate from her choice. Due to geographic distance, privacy concerns, or simply the scale of these systems, each player can only base her decision on local information. I present our algorithm on learning Nash equilibria in convex games and discuss its convergence.

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On System Theoretic Principles for Nash Equilibrium Seeking Dynamics

Lacra Pavel

System Control Group and Photonics Group, University of Toronto, Canada

We consider a set of agents playing a game whose goal is to achieve a collective configuration described by a Nash equilibrium. The setting is non-cooperative in the way actions are taken (each agent minimizes its own individual cost), but collaborative in the sense that agents may share some information with neighbours to compensate for the lack of global information. We show how system theory and passivity properties can be used in the analysis and design of Nash seeking distributed dynamics.

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Event-triggered control for nonlinear systems with time delay

Kexue Zhang

University of Calgary

This talk focuses on the event-triggered control problem of time-delay systems. We present a novel event triggering algorithm with two tunable parameters, based on a Lyapunov-Krasovskii functional result for input-to-state stability. The proposed algorithm ensures the resulting closed-loop systems to be globally asymptotically stable, uniformly bounded, and/or globally attractive for different choices of these parameters. Sufficient conditions on the parameters are derived to exclude Zeno behavior. We also discuss some possible applications of the proposed algorithm on consensus problems of multi-agent systems. This is joint work with Bahman Gharesifard (Queen's University) and Elena Braverman (University of Calgary).

Financial Mathematics 1

Organizer: **Christina Christara, Ken Jackson**

An ϵ-monotone Fourier method for Guaranteed Minimum Withdrawal Benefit (GMWB) as a continuous impulse control problem

Yaowen Lu

School of Mathematics and Physics, University of Queensland, Australia

When modeled as an impulse control problem, the no-arbitrage pricing of Guaranteed Minimum Withdrawal Benefit (GMWB) contracts with continuous withdrawals results in a Hamilton-Jacobi-Bellman quasi-integro-variational inequality (HJB-QVI). We develop a novel ϵ-monotone Fourier method for solving this HJB-QVI problem that achieves monotonicity within an infinitesimal tolerance ϵ. We extend the convergence framework of G. Barles and P.E. Souganidis (Asymptotic Analysis, 4:271–283, 1991), which is originally developed for strictly monotone schemes, to rigorously prove the convergence of numerical solutions to the viscosity solution of the associated HJB-QVI, as a discretization parameter and monotonicity tolerance ϵ approach zero, provided a strong comparison result holds. We study efficient padding techniques and the use of asymptotic solutions in the padding areas to effectively control wrap-around errors. Numerical experiments demonstrate an excellent agreement with benchmark results obtained by finite difference methods and Monte Carlo simulation.

Joint work with Duy Minh Dang, Peter Forsyth, and George Labahn.

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Optimal Execution with Stochastic Delay

Alvaro Cartea

Mathematical Institute, University of Oxford, United Kingdom

We show how traders use marketable limit orders (MLOs) to liquidate a position over a trading window when there is latency in the marketplace. MLOs are liquidity taking orders that specify a price limit and are for immediate execution only; however, if the price limit of the MLO precludes it from being filled, the exchange rejects the trade. We frame our model as an impulse control problem with stochastic latency where the trader controls the times and the price limits of the MLOs sent to the exchange. We show that impatient liquidity takers submit MLOs that may walk the book (capped by the limit price) to increase the probability of filling the trades. On the other hand, patient liquidity takers use speculative MLOs that are only filled if there has been an advantageous move in prices over the latency period. Patient traders who are fast do not use their speed to hit the quotes they observe, nor to finish the execution programme early; they use speed to complete the execution programme with as many speculative MLOs as possible. We use foreign exchange data to implement the random-latency-optimal strategy and to compare it with four benchmarks: execution with deterministic latency, execution with zero latency, time-weighted average price, and execution of the entire order at the best quote in the LOB at the beginning of the trading window. We find that the performances of the random-latency and the deterministic-latency strategies are similar. For patient traders, these two strategies outperform the other three benchmarks by an amount that is greater than the transaction costs paid by liquidity takers in foreign exchange markets. Around news announcements, the value of the outperformance is between two and ten times the value of the transaction costs. The superiority of the latency-optimal strategies is due to both the speculative MLOs that are filled and the price protection of the MLOs.

Joint work with Leandro Sánchez-Betancourt.

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Neural-SDE market models without static arbitrage

Christoph Reisinger

Mathematical Institute, University of Oxford, United Kingdom

Modelling joint dynamics of liquid vanilla options is crucial for arbitrage-free pricing of illiquid derivatives and managing risks of option trade books. This talk presents a nonparametric model for the European options book that is theoretically sound and implementable. We derive a state space for prices which are free from static (or model–independent) arbitrage and study the inference problem where a model is learnt from discrete time series data of stock and option prices. We use neural networks as function approximators for the drift and diffusion of the modelled SDE system, and impose constraints on the neural nets such that arbitrage conditions are preserved. In particular, we give methods to calibrate neural SDE models which are guaranteed to satisfy a set of linear (in)equalities. We validate our approach with numerical experiments using data generated from a Heston stochastic local volatility model.

Joint work with Samuel N. Cohen and Sheng Wang.

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Equilibrium Pricing in Solar Renewable Energy Certificate (SREC) Markets: A Mean Field Game Approach

Dena Firoozi

Department of Decision Sciences, HEC Montreal, Canada

Solar renewable energy certificate (SREC) markets can be viewed through the lens of a large stochastic game with heterogeneous agents, where agents interact through the market price of the certificates. We study this stochastic game by solving the mean-field game (MFG) limit with sub-populations of heterogeneous agents. Our market participants optimize costs accounting for trading frictions, cost of generation, non-linear non-compliance penalty, and generation uncertainty. Moreover, we endogenize SREC price through market clearing. Using techniques from variational analysis, we characterize firms' optimal controls as the solution of McKean-Vlasov (MV) FBSDEs and determine the equilibrium SREC price. We establish the existence and uniqueness of a solution to this MV-FBSDE, and further prove that the MFG strategies have the ϵ-Nash property for the finite player game. Finally, we develop a numerical scheme for solving the MV-FBSDEs and conclude by demonstrating how firms behave in equilibrium using simulated examples.

Joint work with Arvind Shrivats and Sebastian Jaimungal.

Financial Mathematics 2

Organizer: **Christina Christara, Ken Jackson**

Oil market games, nonlinear ODEs, and singularities

Matt Davison

School of Mathematical and Statistical Sciences, Western University, Canada

A piecewise defined system of Hamilton Jacobi Bellman PDE arises from a differential game model in energy markets. A similarity transformation allows this to be reduced to a piecewise defined nonlinear ODE with smooth pasting conditions at internal join points defined from conditions at which producers enter or exit the market.

This interesting system of ODEs requires classical and modern Applied Mathematics tools for its resolution, as it is both deeply nonlinear and involves problematic boundary conditions and for internal moving singularities which, if ignored, can challenge numerical methods.

I will describe our ongoing work to fully understand this system and its numerical solutions.

Joint work with Rob Corless and Junhe Chen.

Portfolio Optimisation within a Wasserstein Ball

Sebastian Jaimungal

Department of Statistics, University of Toronto, Canada

We study the problem of active portfolio management where an investor aims to outperform a benchmark strategy's risk profile while not deviating too far from it. Specifically, an investor considers alternative strategies whose terminal wealth lie within a Wasserstein ball surrounding a benchmark's – being distributionally close ? and that have a specified dependence/copula – tying state-by-state outcomes – to it. The investor then chooses the alternative strategy that minimises a distortion risk measure of terminal wealth. In a general (complete) market model, we prove that an optimal dynamic strategy exists and provide its characterisation through the notion of isotonic projections.

We further propose a simulation approach to calculate the optimal strategy's terminal wealth, making our approach applicable to a wide range of market models. Finally, we illustrate how investors with different copula and risk preferences invest and improve upon the benchmark using the Tail Value-at-Risk, inverse S-shaped, and lower- and upper-tail distortion risk measures as examples. We find that investors' optimal terminal wealth distribution has larger probability masses in regions that reduce their risk measure relative to the benchmark while preserving the benchmark's structure.

Joint work with Silvana Pesenti, U. Toronto.

A Generalized Multi-Level Monte Carlo Method

Tony Ware

Department of Mathematics and Statistics, University of Calgary, Canada

The Multi-Level Monte Carlo (MLMC) method has been applied successfully in a wide range of settings over the last decade or so since its introduction by Giles in 2008. When using only two levels, the method can be viewed as a kind of control-variate approach to variance reduction, and indeed in this form it appeared in the work of Emsermann and Simon in 2002, Kebaier in 2005, and Speight in 2009. In this talk, we describe how the control-variate formulation can be extended to any number of levels, generalizing the MLMC method. We show how this can lead to improvements in efficiency, especially when the coarsest level approximation is actually coarse and relatively inaccurate.

Joint work with my Ph.D. student Yu Li.

A data-driven neural network approach to dynamic factor investing with transaction costs

Pieter van Staden

Cheriton School of Computer Science, University of Waterloo, Canada

We present a data-driven neural network approach to find optimal dynamic (multi-period) factor investing strategies in the presence of transaction costs. The factor investing problem is formulated as a stochastic optimal control problem, which we solve and analyze using two objectives, namely a (i) one-sided quadratic target objective (closely related to dynamic mean-variance optimization), and a (ii) mean - conditional value-at-risk (CVaR) objective. The results are illustrated using a realistic factor investing scenario: we assume that the investor does not allow short-selling or leverage, considers only widely accepted equity factors that are directly and cost-effectively investable in practice, and wishes to allocate wealth to equity factors and bonds simultaneously. We find that a basic portfolio consisting of only a broad equity market index and bonds can be very competitive compared to the corresponding optimal factor portfolios. We also show that the optimal factor portfolios, the composition and performance of which can be very sensitive to the choice of the training data used by the neural network, can lead to out-of-sample investment outcomes that may easily disappoint the investor.

Joint work with Peter Forsyth and Yuying Li.

Scientific Computation 1

Organizer: **Giang Tran, Sander Rhebergen**

Physics-informed neural networks for the shallow-water equations on there sphere

Alexander Bihlo

Department of Mathematics and Statistics, Memorial University of Newfoundland, Canada

We propose the use of physics-informed neural networks for solving the shallow-water equations on the sphere. Physics-informed neural networks are trained to satisfy the differential equations along with the prescribed initial and boundary data, and thus can be seen as an alternative approach to solving differential equations compared to traditional numerical approaches such as finite difference, finite volume or spectral methods. We discuss the training difficulties of physics-informed neural networks for the shallow-water equations on the sphere and propose a simple multi-model approach to tackle test cases of comparatively long time intervals. We illustrate the abilities of the method by solving the most prominent test cases proposed by Williamson et al. [J. Comput. Phys. 102, 211-224, 1992]. This is joint work with Roman O. Popovych.

Mass-conservative and positivity preserving second-order methods for high order parabolic

Yves Bourgault

Department of Mathematics & Statistics, University of Ottawa, Canada

High order parabolic equations, such as Cahn-Hilliard equations, are notoriously difficult to solve numerically because of the fourth order of the spatial differential operator combined with degeneracies and nonlinearities of some of the coefficients. This leads to challenges in designing numerical methods beyond first order is

space and time steps, without sacrifying mass conservation and positivity of the numerical solutions. We consider a class of finite element approximations for fourth-order parabolic equations that can be written as a system of second-order equations by introducing an auxiliary variable. The time-discretization is based on the semi-implicit BDF formulae. In our approach, we first solve a variational problem and then an optimization problem to satisfy the desired physical properties of the solution such as conservation of mass, positivity (non-negativity) of solution and dissipation of energy. The methodology is general and can be applied to a broader set of problems. Numerical results will be presented to illustrate the efficiency and robustness of the approach.

This work is co-authored with Sana Keita and Abdelaziz Beljadid, from uOttawa and UM6P, Morocco.

Variable time-stepping methods for fluid-structure interaction problems

Martina Bukač

Department of Applied & Computational Mathematics & Statistics, University of Notre Dame, USA

In realistic flow problems described by partial differential equations (PDEs), where the dynamics are not known, or in which the variables are changing rapidly, the robust, adaptive time-stepping is central to accurately and efficiently predict the long-term behavior of the solution. This is especially important in the coupled flow problems, such as the fluid-structure interaction (FSI), which often exhibit complex dynamic behavior. While the adaptive spatial mesh refinement techniques are well established and widely used, less attention has been given to the adaptive time-stepping methods for PDEs. We will discuss novel, adaptive, partitioned numerical methods for FSI problems with thick and thin structures. The time integration in the proposed methods is based on the refactorized Cauchy's one-legged 'theta-like' method, which consists of a backward Euler method, where the fluid and structure sub-problems are sub-iterated until convergence, followed by a forward Euler method.The bulk of the computation is done by the backward Euler method, as the forward Euler step is equivalent to (and implemented as) a linear extrapolation. We will present the numerical analysis of the proposed methods showing linear convergence of the sub-iterative process and unconditional stability. The time adaptation strategies will be discussed. The properties of the methods, as well as the selection of the parameters used in the adaptive process, will be explored in numerical examples.

Asymptotic-preserving IMEX-DG methods for a linear kinetic transport model: different reformulations and IMEX strategies

Fengyan Li

Department of Mathematical Sciences, Rensselaer Polytechnic Institute, USA

We consider a linear kinetic transport equation under a diffusive scaling, that has a diffusive equation as the limit when the Knudsen number goes to zero. The equation provides a prototype model to study many systems, including neutronic dynamics and radiation transfer. One type of numerical methods that can simulate such multi-scale models efficiently is the asymptotic preserving (AP) method. Our focus here is on devising accurate AP methods, that are uniformly stable from transport to diffusive regimes, by applying discontinuous Galerkin (DG) methods in space and implicit-explicit (IMEX) Runge-Kutta methods in time. We will present several families of IMEX-DG methods based on different reformulations of the model and different IMEX strategies. Computational complexity and theoretical findings will be discussed, along with some numerical examples.

Scientific Computation 2

Organizer: **Giang Tran, Sander Rhebergen**

Convergence Acceleration for Nonlinear Fixed-Point Methods

Hans De Sterck

Department of Applied Mathematics, University of Waterloo, Canada

Empirical results show that nonlinear convergence acceleration methods such as Anderson Acceleration (AA) or the Nonlinear Generalized Minimal Residual (NGMRES) method may often dramatically speed up the convergence of fixed-point algorithms that are widely used in scientific computing and optimization. However, little is known theoretically that can help us to understand and quantify the asymptotic convergence improvement. We present new results that shed light on this open problem, by considering optimal stationary versions of the acceleration methods that allow us to quantify the convergence improvement using spectral properties of the Jacobian of the fixed-point iteration function, viewed as a nonlinear preconditioner. We illustrate these findings for nonlinear acceleration of the Alternating Least Squares (ALS) method for canonical tensor decomposition and the Alternating Direction Method of Multipliers (ADMM) for optimization problems in machine learning.

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A Machine Learning Framework for Mean Field Games and Optimal Control

Lars Ruthotto

Department of Mathematics, Emory University, USA

We consider the numerical solution of mean field games and optimal control problems whose state space dimension is in the tens or hundreds. In this setting, most existing numerical solvers are affected by the curse of dimensionality (CoD). To mitigate the CoD, we present a machine learning framework that combines the approximation power of neural networks with the scalability of Lagrangian PDE solvers. Specifically, we parameterize the value function with a neural network and train its weights using the objective function with additional penalties that enforce the Hamilton Jacobi Bellman equations. A key benefit of this approach is that no training data is needed, e.g., no numerical solutions to the problem need to be computed before training. We illustrate our approach and its efficacy using numerical experiments. To show the framework's generality, we consider applications such as optimal transport, deep generative modeling, mean field games for crowd motion, and multi-agent optimal control.

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Deep Learning meets Shearlets: Towards Interpretable Image Reconstruction

Gitta Kutyniok

Department of Mathematics, Ludwig-Maximilians-Universität München, Germany

Pure model-based approaches are today often insufficient for solving complex inverse problems in medical imaging. At the same time, methods based on artificial intelligence, in particular, deep neural networks, are extremely successful, often quickly leading to state-of-the-art algorithms. However, pure deep learning

approaches often neglect known and valuable information from the modeling world and suffer from a lack of interpretability.

In this talk, we will develop a conceptual approach by combining the model-based method of sparse regularization by shearlets with the data-driven method of deep learning. Our solvers pay particular attention to the singularity structures of the data. Focussing then on the inverse problem of (limited-angle) computed tomography, we will show that our algorithms significantly outperform previous methodologies, including methods entirely based on deep learning. Finally, we will also touch upon the issue of how to interpret such algorithms, and present a novel, state-of-the-art explainability method based on information theory.

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Data-driven solutions to inverse problems

Carola-Bibiane Schönlieb

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom

Inverse problems are about the reconstruction of an unknown physical quantity from indirect measurements. In imaging, they appear in a variety of places, from medical imaging, for instance, MRI or CT, to remote sensing, for instance, Radar, to material sciences and molecular biology, for instance, electron microscopy. Here, imaging is a tool for looking inside specimens, resolving structures beyond the scale visible to the naked eye, and to quantify them. It is a means for diagnosis, prediction, and discovery.

Most inverse problems of interest are ill-posed and require appropriate mathematical treatment for recovering meaningful solutions. Classically, inversion approaches are derived almost conclusively in a knowledge driven manner, constituting handcrafted mathematical models. Examples include variational regularization methods with Tikhonov regularization, the total variation and several sparsity-promoting regularizers such as the L1 norm of Wavelet coefficients of the solution. While such handcrafted approaches deliver mathematically rigorous and computationally robust solutions to inverse problems, they are also limited by our ability to model solution properties accurately and to realise these approaches in a computationally efficient manner.

Recently, a new paradigm has been introduced to the regularization of inverse problems, which derives solutions to inverse problems in a data driven way. Here, the inversion approach is not mathematically modelled in the classical sense, but modelled by highly over-parametrised models, typically deep neural networks, that are adapted to the inverse problems at hand by appropriately selected (and usually plenty of) training data. Current approaches that follow this new paradigm distinguish themselves through solution accuracies paired with computational efficiency that were previously unconceivable. In this talk, I will provide a glimpse into such deep learning approaches and some of their mathematical properties. I will finish with open problems and future research perspectives.

Fluid Dynamics/Climate 1

Organizer: **Michael Waite, Marek Stastna**

Filling in the Map: Understanding Arctic Ocean mixing space-time geography & its implications

Stephanie Waterman

Department of Earth, Ocean & Atmospheric Sciences, University of British Columbia, Canada

The rates and mechanisms of ocean mixing are important controls on how the oceans function; yet, our understanding of mixing in the ocean is significantly limited by complex variability in mixing rates and processes and by a scarcity of direct observations. In the Arctic Ocean, the challenges are significant: mixing measurements are especially sparse and latitude, ice, and stratification make the mixing environment unique. In this talk, I'll discuss various ways we are mapping Arctic Ocean mixing rates and deriving insights into what sets mixing space-time geography using pan-Arctic measurements from autonomous instrument platforms and the archived data record. I'll also show results from our experiments with realistic ocean models to argue that this map matters both to our understanding of Arctic Ocean functioning and our ability to make robust predictions of climate change.

Characterizing internal waves and mesoscale eddies at four deep ocean sites

Ruth Musgrave[a], Elisabeth Fine[b], Richard Krishfield[b], John Toole[b]

[a]Department of Oceanography, Dalhousie University, Canada
[b]Woods Hole Oceanographic Institution, USA

We present observations of currents and density from full-depth, multi-year moored measurements at deep-ocean sites in the Irminger Sea, Argentine Basin, Southern Ocean and North Pacific obtained by the Ocean Observatory Initiative supported by the U.S. National Science Foundation. Each site represents a distinct physical oceanographic environment characterized by stratification, wind stress, eddy kinetic energy, tidal amplitude and local bathymetry. This investigation, currently at a preliminary stage, focusses on the dynamics of subinertial, internal tide and near-inertial processes, comparing observations to linear theory that describes the vertical structures and propagation characteristics of subinertial motions and superinertial internal waves.

We find examples of both locally- and remotely-generated downward-propagating near-inertial waves. Locally generated waves have intrinsic frequencies both slightly above and below the local Coriolis frequency, and are associated with depth-coherent surface layer oscillations. Internal tides are common across all sites but with varying degrees of intermittency and vertical structure that include both low modes and upward propagating beams. We explore the consistency of observed internal wave properties compared to linear theory, and contrast the vertical structure of subinertial modes with predictions in the presence of either flat or sloped bottom bathymetry.

Waves over Topography in a Rotating World: Upwelling induced by coastal trapped waves over a submarine canyon

Gonzalo Saldias[a], Karina Ramos Musalem[b], **Susan Allen**[c]

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[b]National University of Mexico (UNAM), Mexico City, Mexico
[c]Department of Earth, Ocean & Atmospheric Sciences, University of British Columbia, Canada

The various dynamics that drive upwelling of nutrient rich waters in the coastal ocean is a classic physical oceanography problem with large ecological impacts. Here we return to the response to passing over a submarine canyon of Coastal Trapped Waves (CTWs) which are stratified Kelvin waves mixed with topographic Rossby waves. New observational evidence suggests much larger upwelling over BioBio Canyon than expected. Here, we use idealized numerical experiments to assess the role of CTWs in promoting the onshore transport of deeper waters onto the continental shelf. The experiments are forced with a 7-day

period CTW, much longer than the inertial period. However, as the flow response over a canyon is partially advective, 7-days is not long enough for the CTW response to be simply upwelling followed by downwelling. Overall, there is accumulated upwelled water in time which is advected along the coast in the direction the wave is propagating, on the opposite side of the canyon to the upwelled water produced by classic, steady upwelling over a canyon.

Balance and imbalance in rotating stratified turbulence

Peter Bartello

Departments of Mathematics & Statistics and Atmospheric & Oceanic Sciences, McGill University, Canada

While it is well-established that the frequency disparity between vortical and wave motions is key to understanding the simplified quasigeostrophic limit (strong rotation and stratification), the starting point for this work is that it is now generally accepted there is no such asymptotic frequency disparity in stratified turbulence without rotation. This undermines the entire notion of simplified balance dynamics at scales well below the baroclinic eddy scale in both atmosphere and ocean. It remains to ask what happens in between these two limits, long held as the prevailing dynamics between deformation-scale eddies and the effective depth of the fluid, below which isotropy is potentially recovered. To do this, techniques from numerical weather prediction were borrowed in order to explore numerically the nonhydrostatic Boussinesq equations starting from initial conditions that are within our current fuzzy notion of balance for a variety of rotation rates and density stratifications. It is found that evolution is spontaneously away from this balance in the small scales, and from steep to much more shallow energy spectra. It will be argued these results are both robust to uncertainties in the definition of balance and are consistent with observations. The latter have alternatively been explained as resulting from surface quasigeostrophic flow on the tropopause (where aircraft observations are primarily taken) and from a layer-wise 2-D inverse energy cascade from small-scale convection. While both have been discredited, it remains to determine the effect of the convective energy source within our current understanding. Some preliminary work on this will be discussed.

Fluid Dynamics/Climate 2

Organizer: **Michael Waite, Marek Stastna**

Ekman-inertial instability

Nicolas Grisouard

Department of Physics, University of Toronto, Canada

We report on an instability arising in sub-surface, laterally sheared geostrophic flows. When the lateral shear of a horizontal flow in geostrophic balance has a sign opposite to the Coriolis parameter and exceeds it in magnitude, embedded perturbations are subjected to inertial instability, albeit modified by viscosity. When the perturbation is a step-like disturbance on the surface of the fluid, the initial response is akin to a Stokes problem, with an initial flow aligned with the initial perturbation. The perturbation then grows quasi-inertially, rotation deflecting the velocity vector, which adopts a well-defined angle with the mean flow, and viscous stresses, transferring horizontal momentum downward. The combination of rotational and viscous effects in the dynamics of inertial instability prompts us to call this process "Ekman-inertial

instability." While the perturbation initially grows super-inertially, the growth rate then becomes sub-inertial, eventually tending back to the inertial value. The same process repeats downward as time progresses. Ekman-inertial transport aligns with the asymptotic orientation of the flow and grows exactly inertially with time once the initial disturbance has passed. Because of the strongly super-inertial initial growth rate, this instability might compete favourably against other instabilities arising in ocean fronts. In the presence of baroclinicity, buoyancy is advected during Ekman-inertial instability like a passive scalar. In most cases, this leads to frontogenesis, though frontolysis is also possible. In all cases, Ekman inertial instability would extract potential energy from a front. It, combined with its initially large growth rate, would violate some theoretically predicted impacts of negative-potential-vorticity ageostrophic instabilities on baroclinic fronts.

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Inertial instability in a tropical oceanic jet

Francis J. Poulin, Matthew Harris, Kevin G. Lamb

Department of Applied Mathematics, University of Waterloo, Canada

Inertial instability is one of the mechanisms through which oceanic jets can break up and form vortical motions. This instability tends to be faster growing than barotropic and baroclinic instabilities and has the effect of mixing the Potential Vorticity of the fluid, to yield a resulting flow that is stable.

In this talk we investigate the dynamics of a barotropic jet in a weakly stratified, tropical ocean subject to both traditional and non-traditional Coriolis pseudo-forces. First, we numerically compute the linear stability characteristics for a range of parameters to determine how the number of unstable modes increases significantly with decreasing stratification. This also reveals that the non-traditional term has a significant impact on the spatial structure of the unstable modes in that they are always tilted in the vertical. Second, we investigate the nonlinear evolution of these modes using the library Oceananigans.jl. This shows that the states that occur after nonlinear equilibration differ significantly based on the background stratification.

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Using stochastic models to improve the representation of clouds and large-scale tropical wave dynamics in climate models

Boualem Khouider

Department of Mathematics and Statistics, University of Victoria, Canada

Cumulus parameterization (CP) in state-of-the-art global climate models (GCM) is based on the quasi-equilibrium assumption (QEA), which views convection as the action of an ensemble of cumulus clouds, in a state of equilibrium with respect to a slowly varying atmospheric large scale state. This view is not compatible with the organization and dynamical interactions across multiple scales of cloud systems in the tropics and progress in this research area was slow over decades despite the widely recognized major shortcomings. The last two decades have seen a surge of novel ideas on how to represent key physical processes of moist convection-large-scale interaction to overcome the QEA. This led to new breakthroughs in CP. The stochastic multicloud model (SMCM) CP was in particular mimics the multiple cloud types that characterize organized tropical convection. Here, the SMCM is used to modify the Zhang-McFarlane (ZM) CP by changing the way the bulk mass flux is calculated. We build in a stochastic ensemble of plumes characterized by randomly varying detrainment level distributions based on the cloud area fraction (CAF) predicted by the SMCM. The SMCM is here extended to include shallow cumulus clouds resulting in a unified shallow-deep CP. The new stochastic multicloud plume CP is validated against the control ZM scheme in the context of the single column Community Climate Model of the National Center for Atmospheric Research

using six test-cases including both tropical ocean and midladitude land convection. The use of stochastic parameterization to account for the uncertainty in model error is demonstrated.

Global temperature control on the Dansgaard-Oeschger Oscillations

Louis-Philippe Nadeau

Institut des sciences de la mer de Rimouski, Université du Québec à Rimouski, Canada

Dansgaard?Oeschger (DO) events are abrupt climate variations that occurred during the last glacial interval. They are characterized by (i) a sawtooth-shaped Northern Hemisphere high-latitude temperatures, (ii) a ?bipolar seesaw? connection between the climate variability in the Northern and Southern Hemispheres, and (iii) a variation in the frequency of DO events during the glacial period. Most theories that have been proposed to explain the DO cycles suggest an interplay between the Meridional Overturning Circulation (MOC), the ice sheets/shelves, and sea ice cover, but the exact combination of these physical mechanisms is still debated. Here, we develop a simple predictive framework that captures the main characteristics of the DO cycles using a minimal number of physical variables. The robustness of the framework is tested against equilibrium solutions of a 3D ocean General Circulation Model. In both models, a transition between present-day-like climate and glacial-like climate is observed as the global surface temperature is decreased. Global temperature alone controls the frequency of the oscillations, with a key role of North Atlantic sea ice in controlling the climate variability. A continuous transition is observed between mainly ice-free (interstadial) conditions in warm climates and mainly ice-covered (stadial) conditions in cold climates, with oscillatory regimes between these two extreme cases. The average stadial period increases with cooling global temperatures, while the average interstadial period sharply decreases. Our results show that the main features of the oscillations can be explained with simple physical mechanisms of a coupled ocean-seaice system under time-constant forcing.

Data Science/Machine Learning 1

Organizer: **Yaoling Yu, Kimon Fountoulakis**

From local structures to size generalization in graph neural networks

Haggai Maron

NVIDIA Research

Graph neural networks (GNNs) can process graphs of different sizes, but their ability to generalize across sizes, specifically from small to large graphs, is still not well understood. In this talk, we will identify an important type of data where generalization from small to large graphs is challenging: graph distributions for which the local structure depends on the graph size. This effect occurs in multiple important graph learning domains, including social and biological networks. We first prove that when there is a difference between the local structures, GNNs are not guaranteed to generalize across sizes: there are "bad" global minima that do well on small graphs but fail on large graphs. We will then study the size-generalization problem empirically and demonstrate that when there is a discrepancy in local structure, GNNs tend to converge to non-generalizing solutions in practice. Finally, I will suggest two approaches for improving size generalization, motivated by our findings.

Persistent message passing

Petar Veličković

DeepMind

Most GNNs are designed with Markovian querying in mind: latent representations are overwritten in every step, and the last representation is used to answer queries. This overloads GNNs' latents, as all past snapshots of the data must be represented within them.

We propose Persistent Message Passing (PMP), replacing overwriting with persisting: when updating a node's state, a copy of that node is preserved for later use. To avoid excessive memory usage, PMP has a mechanism to select which nodes to persist. PMP effectively provides GNNs with an episodic memory of their previous computations. Further, it aligns with the broad class of persistent data structures, which further expands the space of general-purpose algorithms that can be neurally executed. We show on dynamic range querying that our method provides significant benefits to overwriting-based GNNs, both in- and out-of-distribution.

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On the generalization of graph neural networks and their applications in probabilistic inference

Renjie Liao

Google Brain and Vector Institute

Graph neural networks (GNNs) recently became popular in handling graph-structured data. In this talk, I will discuss my work which tried to understand the generalization ability of GNNs and apply them to learning probabilistic inference algorithms.

First, we show generalization bounds for the two primary classes of GNNs, namely graph convolutional networks (GCNs) and message passing GNNs (MPGNNs), via a PAC-Bayesian approach. Our result reveals that the maximum node degree and spectral norm of the weights govern the generalization bounds of both models. For MPGNNs, our PAC-Bayes bound improves over the Rademacher complexity-based bound, showing a tighter dependency on the maximum node degree and the maximum hidden dimension.

Then we will introduce how GNNs can be used for probabilistic inference, i.e., estimating the marginal or maximum-a-posterior probabilities. We demonstrate that GNNs substantially outperform belief propagation on loopy graphs. Our learned message-passing algorithms generalize out of the training set to larger graphs and graphs with different structures.

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Graph convolution for semi-supervised classification: improved linear separability and out-of-distribution generalization

Kimon Fountoulakis

Cheriton School of Computer Science, University of Waterloo, Canada

Recently there has been increased interest in semi-supervised classification in the presence of graphical information. A new class of learning models has emerged that relies, at its most basic level, on classifying the data after first applying a graph convolution. To understand the merits of this approach, we study the classification of a mixture of Gaussians, where the data corresponds to the node attributes of a stochastic block model. We show that graph convolution extends the regime in which the data is linearly separable by a factor of roughly 1/sqrt(D), where D is the expected degree of a node, as compared to the mixture model data on its own. Furthermore, we find that the linear classifier obtained by minimizing the cross-entropy loss after the graph convolution generalizes to out-of-distribution data where the unseen data can have different intra- and inter-class edge probabilities from the training data.

Data Science/Machine Learning 2

Organizer: **Yaoling Yu, Kimon Fountoulakis**

Homeomorphic-invariance of EM: non-asymptotic convergence in KL divergence for exponential families via mirror descent

Mark Schmidt

Department of Computer Science, University of British Columbia, Canada

Expectation maximization (EM) is the default algorithm for fitting probabilistic models with missing or latent variables, yet we lack a full understanding of its non-asymptotic convergence properties. Previous works show results along the lines of "EM converges at least as fast as gradient descent" by assuming the conditions for the convergence of gradient descent apply to EM. This approach is not only loose, in that it does not capture that EM can make more progress than a gradient step, but the assumptions fail to hold for textbook examples of EM like Gaussian mixtures. In this work we first show that for the common setting of exponential family distributions, viewing EM as a mirror descent algorithm leads to convergence rates in Kullback-Leibler (KL) divergence. Then, we show how the KL divergence is related to first-order stationarity via Bregman divergences. In contrast to previous works, the analysis is invariant to the choice of parametrization and holds with minimal assumptions. We also show applications of these ideas to local linear (and superlinear) convergence rates, generalized EM, and non-exponential family distributions.

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On the (un-)avoidability of adversarial examples

Ruth Urner

Department of Electrical Engineering and Computer Science, York University, Canada

The phenomenon of adversarial examples in deep learning models has caused substantial concern over their reliability. While many deep neural networks have shown impressive performance in terms of predictive accuracy, it has been shown that in many instances an imperceptible perturbation can falsely flip the network's prediction. In recent years, we have seen a surge of research studies on this phenomenon. On the practical side these have taken the form of a race between developments of attacks and defenses. On the theoretical end, many studies have highlighted unexpected gaps in computational and statistical complexity as well as trade-offs with accuracy induced by requirements of adversarial loss minimization. In this talk, I will review some of these results from recent research. I will then argue that many undesirable properties occurring in the study of learning under adversarial perturbations are artifacts of using an unsuitable definition of adversarial robustness. I will outline some sufficient conditions for closing the sample complexity gaps. Then, I will argue that robustness should be redefined as a locally adaptive requirement and discuss effects of this novel perspective.

Based on joint work with Hassan Ashtiani, Vinayak Pathak and Sadia Chowdhury.

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A generalized objective for off-policy value estimation in reinforcement learning

Martha White

Department of Computing Science, University of Alberta, Canada

Many reinforcement learning algorithms rely on value estimation. However, the most widely used algorithms – namely temporal difference algorithms – can diverge under both off-policy sampling and nonlinear function approximation. Many algorithms have been developed for off-policy value estimation which are sound under linear function approximation, based on the linear mean-squared projected Bellman error (PBE). Extending these methods to the non-linear case has been largely unsuccessful. Recently, several methods have been introduced that approximate a different objective, called the mean-squared Bellman error (BE), which naturally facilitates nonlinear approximation. In this work, we build on these insights and introduce a new generalized PBE, that extends the linear PBE to the nonlinear setting. We show how this generalized objective unifies previous work, including previous theory, and obtain new bounds for the value error of the solutions of the generalized objective. We derive an easy-to-use, but sound, algorithm to minimize the generalized objective which is more stable across runs, is less sensitive to hyperparameters, and performs favorably across four control domains with neural network function approximation.

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Certified robustness of graph convolution networks for graph classification under topological attacks

Xinhua Zhang

Department of Computer Science, University of Illinois at Chicago, USA

Graph convolution networks (GCNs) have become effective models for graph classification. Similar to many deep networks, GCNs are vulnerable to adversarial attacks on graph topology and node attributes. Recently, a number of effective attack and defense algorithms have been designed, but no certificate of robustness has been developed for GCN-based graph classification under topological perturbations with both local and global budgets. In this talk, we propose the first certificate for this problem. Our method is based on Lagrange dualization and convex envelope, which result in tight approximation bounds that are efficiently computable by dynamic programming. When used in conjunction with robust training, it allows an increased number of graphs to be certified as robust.

Mini-Symposia

New quantitative approaches to understand hematopoietic clonality and leukemogenesis in acute myeloid leukemia

Organizer: **Morgan Craig**

Opposing evolutionary pressures drive clonal evolution and health outcomes in the aging blood system

Kimberly Skead[a,b,c], Armande Ang Houle[a,b], Sagi Abelson[a,b], Mawusse Agbessi[a,b], Vanessa Bruat[a,b], Boxi Lin[a], David Soave[a,d], Liran Shlush[e], Stephen Wright[f], John Dick[a,b,g], Quaid Morris[a,b,c,h,i], Philip Awadalla[a,b,j]

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A small population of hematopoietic stem cells continuously reconstitutes our immune system. As we age, these cells accumulate somatic mutations; some of which provide selection advantages and increase in frequency in peripheral blood. This process of positive selection, termed age-related clonal hematopoiesis (ARCH), is associated with increased risk for blood malignancies, like acute myeloid leukemia (AML). However, it is unclear why some people with known AML driver mutations do not progress to AML. Here, we examine if negative selection plays a role in AML progression by modelling the interplay of positive and negative selective processes. Using a novel approach combining deep learning and population genetics, we detect signatures of negative selection using deeply sequenced blood samples from 92 pre-AML individuals and 385 controls. We find that the proportion of passenger to driver mutations is critical in determining if the selective advantage conferred by a driver mutation is able to overwhelm negative selection acting on passenger mutations and allow disease-predisposing clones to rise to dominance. A subset of genes are enriched for mutations in individuals exhibiting purifying selection suggesting these mutations might confer a protective role against ARCH. Through exploring non driver-centric models of evolution, we show how different classes of evolution shape hematopoietic dynamics which may better inform disease prediction and unveil novel therapeutic targets.

Clonal hematopoiesis is accelerated by atherosclerosis

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Hematopoietic stem cells produce all of the body?s blood cells. During clonal hematopoiesis, individual HSCs contribute inordinately to certain types of white blood cells. Though clonal hematopoiesis is not always detrimental to health, it is also associated with blood cancers and atherosclerosis (a build-up of plaque in the arteries). Whether atherosclerosis causes clonal hematopoiesis or clonal hematopoiesis causes atherosclerosis (or a combination of both) is still poorly defined. To better understand this association, we constructed a mathematical model of division and production in the hematopoietic stem cell compartment and neutrophil/monocyte lineages. We found that increased stem cell proliferation increases somatic evolution and clonal expansions with driver mutations. We validated our predictions in vivo using atherosclerotic and sleep fractionated mouse models. Together, our findings suggest a vicious cycle in atherosclerosis wherein increased hematopoietic stem cell division contributes to the association between cardiovascular disease and clonal hematopoiesis.

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How cancer stem cell properties shape clonal evolution and disease dynamics in acute myeloid leukemia - insights from mathematical modeling

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Acute myeloid leukemia is one of the most aggressive cancers. The disease is driven by a small population of so-called leukemic stem cells (LSC) that give rise to the malignant cell bulk and trigger relapse. The malignant cell bulk in each individual patient is composed of multiple clones carrying different subsets of mutations. Due to selection processes and mutation acquisition the abundance of the different clones changes over time. We propose a combination of non-linear dynamical systems models, integro-differential equations models, stochastic simulations and patient data to study how LSC properties evolve due to clonal selection and mutation. The models allow to simulate intra-patient clonal competition and to track the mutational history of the virtual clones. This provides insights in the following questions: How do the leukemic stem cell properties such as proliferation rate or self-renewal probability (the probability that progeny of stem cells

are again stem cells) differ in clones arising early during the disease compared to clones arising late during the disease? Which cell properties are linked to short-term expansion or long-term persistence of a clone? What is the impact of leukemic stem cell and leukemic non-stem cell properties on disease progression? What is the impact of the micro-environment and of systemic signals on leukemic stem cell selection? What can we learn from genetic data? What can bulk sequencing data tell us about disease dynamics?

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Mathematical modelling of the pre-leukemic phase of AML to evaluate clonal reduction therapeutic strategies

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Acute myeloid leukemia (AML) is an aggressive blood cancer subtype characterized by the uncontrolled proliferation of myeloblasts in the bone marrow and the blood. While rare, this disease has one of the highest mortality rates of any leukemias. The inefficiency of standard therapies, which target leukemic cells directly, highlights the need for a new approach to treating AML. Previous studies identified a premalignant phase preceding the onset of AML orchestrated by pre-leukemic stem cells (pre-LSCs). Pre-LSCs outcompete healthy hematopoietic stem cells and allow for AML to develop through their clonal expansion and the acquisition of secondary mutations. More recently, studies have suggested that different approved medications target pre-LSCs. These clonal reduction strategies could completely prevent the evolution of AML; however a better understanding of their impact on hematopoiesis is required. In response, we developed a Moran model of hematopoietic stem cells dynamics in the pre-leukemic phase. To this model, we integrated population pharmacokinetic-pharmacodynamics (PK-PD) models to investigate the clonal reduction potential of several candidate drugs. Our results suggest that three cardiac glycosides (proscillaridin A, digoxin and ouabain) reduce the expansion of premalignant stem cells through a decrease in pre-LSC viability, underlining the prospect of these treatments for AML.

Numerical methods in muscle modelling and its applications 1

Organizer: **Sebastian Dominguez, Raymond Spiteri**

Numerical simulation of cardiac electrophysiology based on representation of individual cells in the EMI model

Aslak Tveito

Department of Computational Physiology, Simula Research Laboratory

Numerical simulations are extensively used to understand cardiac electrophysiology. Classically, the simulations were based on systems of ordinary differential equations modeling the action potential of a single cell. Later, the electrochemical waves in cardiac tissue were modeled using either the Monodomain model or the Bidomain model. In these models, the intracellular space of the cells, the membrane of the cells and the extracellular space were assumed to exist everywhere in the tissue. This represented an enormous

simplification of the physiology, but the models became very popular and yielded interesting results. The models have been used to study many important questions in electrophysiology; the conduction velocity, the effect of electrical shocks (defibrillation), the effect of ischemia, the effect of scar tissue and so on.

A major weakness of the Monodomain and Bidomain models is that the cell is not part of the model. Therefore, the detailed dynamics going on in the vicinity of each cell cannot be studied using these models. This reduces the applicability of these models when it is of interest to analyze electrophysiology at the level of individual cells. Over the past few years, a different approach has been developed. In this model the extracellular space (E), the cell membrane (M) and the intracellular space (I) are explicitly present, and this approach is therefore referred to as the EMI model. In this talk, we will show examples of application of the EMI model and discuss some of the computational challenges using this model. In short, classical models represent cardiac tissue on a millimeter scale and EMI represent the tissue on a micrometer scale. This opens great opportunities for detailed analysis of fine scale electrophysiology, but it also implies huge computational challenges.

The Simulation of Long QT Syndrome using the Extracellular-Membrane-Intracellular Model

Joyce Reimer

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The Extracellular-Membrane-Intracellular (EMI) model describes the spread of action potentials in cardiac muscle. In defining the membrane explicitly, it is able to offer a highly detailed representation of cardiac activity, resolved at the subcellular level. This level of detail offers the potential to produce highly physiologically accurate simulations, but it also poses an intense computational challenge; as the number of cells is increased, the problem size scales up quickly. The existence of a membrane domain in the EMI model makes it an excellent candidate for modelling channelopathies—diseases of the ion channels that are found on the membrane. One of these channelopathies that we have modelled using the EMI approach is Long QT Syndrome 1, a potentially fatal arrhythmogenic disease in which the activity of the slow potassium current, I_{Ks}, is affected. To explore the high computational demands of the EMI model, three systems of increasingly greater numbers of cells are solved and examined for emerging differences in output in order to determine the appropriate problem size for observing the channelopathy. In this presentation, the results of these simulations are presented and analyzed.

Comparing new second-order operator-splitting methods with Strang

Siqi Wei

Department of Mathematics and Statistics, University of Saskatchewan, Canada

The Strang operator-splitting method has been a popular second-order method thanks to its elegant coefficients. New operator-splitting methods have been derived to maximize stability. This potentially allows a problem to be solved with a larger time step, hence reducing the simulation duration. The coefficients of these new methods depending on the underlying Runge–Kutta methods used to integrate each operator.

In this talk, we will go through the development of a pair of operator-splitting methods derived based on stability optimization and the implementation of a general operator-splitting method in Chaste (Cancer, Heart and Soft Tissue Environment). We will compare the performance of the new methods with Strang using the bidomain and monodomain models.

Towards generic temporal operator splitting methods in deal.ii

Kevin Green

Department of Computer Science, University of Saskatchewan

Temporal operator splitting has shown its usefulness when dealing with multi-physics problems. Partitioning multi-physics problems into sub-problems that each individually allow for optimized integration methods has the potential to drastically decrease the real-time duration of a simulation. Optimization of partitioning and sub-problem integration methods is generally impossible a priori, motivating the need for an easily configurable approach to temporal operator splitting.

Motivated additionally by problems in cardiac electrophysiology—in particular the extracellular-membrane-intracellular (EMI) model—this talk discusses recent progress in adding a generic interface to temporal operator splitting methods to the deal.ii finite element library. Discussion will focus on useful structure in the implementation of efficient, extensible time-integration classes, as well as on application examples both in and out of the realm of cardiac electrophysiology.

Young Canadian Researchers – Contributions to Mathematical Modelling in Public Policy 1

Organizer: **Monica Cojocaru, Zahra Mohammadi, Darren Flynn-Primrose**

Re-examination of the impact of non-pharmaceutical interventions and media coverage on the COVID- 19 outbreak in Wuhan City

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In this work, based on the classic Kermack-McKendrick SIR model, we propose an ordinary differential equation model to re-examine the COVID-19 epidemics in Wuhan city where this disease initially broke out. The focus is on the impact of all those major non-pharmaceutical interventions implemented by the local public health authorities and government, to see what roles they played in successfully controlling the epidemic. We use the data publicly available to estimate the model parameters, then explore the impact of those factors in their strengths and timings. The results can help people review the responses to the COVID-19 outbreak in Wuhan, while the proposed model also offers a framework for studying epidemics of COVID-19 and/or other similar diseases in other places and accordingly helping people better prepare for a possible future outbreak of similar diseases.

An Age-stratified transmission model of COVID- 19 in Ontario with Google mobility

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As of July 5th, 2020, there have been over 11.5 million worldwide cases of COVID-19, including over 100 000 in Ontario. Many groups have taken different approaches to modeling the spread of this pandemic. We propose our approach to modelling COVID-19 in Ontario, extend- ing the classic SIR compartmental model by introducing three novel components. First, we incorporate age stratification into our popula- tion structure, distinguishing between 0-19 year olds, 20-59 year olds, and individuals aged 60+. Secondly, we apply the age stratified con- tact rate matrix for Canada found by Prem, Cook, Jit (2017) to our model. Lastly, we introduce several additional compartments to the SEIR model, distinguishing between presymptomatic, asymptomatic and symptomatic infectious individuals. Using a derivative-free opti- mization algorithm, we solve for the optimal effective contact rate to fit our model to reported cases of COVID-19 in Ontario by (italicized) case onset date, as reported by Ontario?s integrated Public Health Information System (iPHIS). In addition, we explore the effects of using Google Mobility data to motivate contact rate, allowing us to solve for transmission rate, decoupling it from contact rate. As mobility changes through various phases of lockdown and social distancing measures, we explore the change on transmission due to external factors such as tem- perature changes, additional hygienic measures like hand washing and sanitation, and mask use.

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Estimating COVID-19 cases and deaths prevented by non-pharmaceutical interventions in 2020-2021, and the impact of individual actions: a retrospective model-based analysis

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Simulation models from the early COVID-19 pandemic highlighted the urgency of applying non-pharmaceutical interventions (NPIs), but had limited empirical data. Here we use data from 2020-2021 to retrospectively model the impact of NPIs. Our model represents age groups and census divisions in Ontario, Canada, and is parameterised with epidemiological, testing, demographic, travel, and mobility data. The model captures how individuals adopt NPIs in response to reported cases. Combined school/workplace closure and individual NPI adoption reduced the number of deaths in the best-case scenario for the case fatality rate (CFR) from 174,411 [CI: 168,022, 180,644] to 3,383 [CI: 3,295, 3,483] in the Spring 2020 wave. In the Fall 2020/Winter 2021 wave, the introduction of NPIs in workplaces/schools reduced the number of deaths from 17,291 [CI: 16,268, 18,379] to 4,167 [CI: 4,117, 4,217]. Deaths were several times higher in the worst-case CFR scenario. Each additional 7-11 (resp. 285-452) individuals who adopted NPIs in the first wave prevented one additional infection (resp., death). Our results show that the adoption of NPIs prevented a public health catastrophe.

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Towards an agent based model of a child care facility and the problem of validating simulated data

D. Flynn-Primrose[a], N. Hoover[a], Z. Mohammadi[a], A. Hung[c], J. Lee[c], M. Tomovici[c], E. W. Thommes[a,b], D. Neame[c], M. G. Cojocaru[a]

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Unlike differential equation models, agent based models (ABM) are able to readily introduce heterogeneity into individual attributes and are tailored to reflect the emerging behaviour, at population level, resulting

from the agent-to-agent and/or agent-to-environment interactions. In this lecture, we describe an ABM model of a child care center modelled after the Child Care and Learning Center (CCLC) at the University of Guelph, in Guelph, ON, Canada. We elaborate on the collection of empirical data as well as the statistical tools employed to analyze it. Additionally, we provide details regarding the basic structure of the mode and we discuss the method used to validate our simulated results. We conclude with a discussion of our results and a few remarks regarding future possibilities.

Mathematical Modelling of COVID-19 Transmission and Mitigation Strategies: Efforts to End the Pandemic 1

Organizer: **Jude Kong, Elena Aruffo**

Modelling the COVID-19 pandemic in South Africa: the role of AI

Bruce Mellado

School of Physics, University of the Witwatersrand, South Africa

In this presentation work performed by the Gauteng Province Premier COVID-19 Advisory Committee in data analysis, modelling, predictions and vaccine roll-out straggles. The use of Artificial Intelligence through Machine Learning in devising smart algorithms will be highlighted. The challenges of interfacing advanced analytics with advising policy-makers will also be discussed.

A model that incorporates non-pharmaceutical interventions, human behavioural characteristics and vaccination to investigate the long term dynamics of SARS-CoV-2 virus disease in a variable human population

Ngwa Gideon

Department of Mathematics, University of Buea, Cameroon

The use of face masks and adherence to general social distancing protocols, personal hygiene, etc, are methods that have been pushed forward by many nations to curb the spread of the SARS-Cov-2 virus. It has been established that these intervention methods can also potentially reduce the severity of a new infection, especially if the viral particles a healthy individual comes in contact with is minimal. Additionally, a well enacted contact tracing procedure can also help identify potential new cases which, in the event that the identified individuals adhere to the social distancing and mask wearing intervention strategies, and self-quarantine could potentially reduce or eliminate the SARS-Cov-2 viral spread to healthy individuals. Human behavioural characteristics, including personal choices of individuals, are crucial in pushing forward a vaccination agenda as well as the proper implementation of non-pharmaceutical intervention strategies. In many African communities, belief systems play an important role and can hinder the effective roll out of intervention strategies including vaccination. Here, we present a long-term mathematical model that was developed and used to understand how the combinations of the aforementioned intervention methods-contact tracing, mask wearing, and self-quarantining can impact the long term dynamics of SARS-CoV-2 spread in varying human populations.

Time between infections versus time between symptom onset in COVID-19: implications for estimating the reproduction number

Jesse Knight

University of Toronto, Canada

The effective reproduction number Re(t) is the average number of new infections directly generated from each existing infection under the conditions at time t. Re(t) can be calculated from the number of daily infections and the time between subsequent infections—the infection-infection distribution, G(t). The infection-infection distribution G(t) is often approximated by the symptom-symptom distribution S(t), because the time of infection can be difficult to determine. However, if the time between infection and symptom onset—the infection-symptom distribution H(t)—varies substantially, then the infectee can develop symptoms before the infector and S(t) can be negative, such as in the case of COVID-19. In this case, it may be improper to approximate G(t) with S(t). Given parametric equations for the symptom-symptom distribution S(t) and the infection-symptom distribution H(t), we develop a method to recover the infection-infection distribution G(t) using approximate deconvolution. We then compare estimates of Re(t) for the Greater Toronto Area using G(t) to those using S(t); two definitions of S(t) are considered, which do and do not allow negative values, respectively. We estimated the time between COVID-19 infections G(t) to be Gamma-distributed with mean 4.08 and standard deviation 3.19 days. The negative-permitting distribution S(t) had equal mean but larger variance than G(t), resulting in underestimation of Re(t) relative to G(t), whereas the non-negative S(t) had similar variance but larger mean, resulting in overestimation of Re(t). Approximation of the infection-infection distribution G(t) with the symptom-symptom distribution S(t) may result in biased estimates of the effective reproduction number R(t). The infection-infection distribution G(t) can also be understood as the distribution of infectiousness; thus accurately distinguishing G(t) from S(t) may also have implications for isolation interventions. Future work should explore possible correlation between S(t), H(t), and G(t) and estimation of confidence intervals for distribution parameters.

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Some Mathematical Models of COVID-19 Transmission and the Role of Protective Measures

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Disease transmission is studied through disciplines like epidemiology, applied mathematics and statistics. Mathematical models that are simulated for transmission have implications in public and personal health challenges. The SIR (Susceptible-Infected-Removed) model uses a compartmental approach including dynamic and nonlinear behavior of transmission through three factors: susceptible, infected, and removed (recovered and deceased) individuals. We use analytical methods, incorporating computer algebra software and the Lambert W Function, to propose a framework to study solutions of the SIR model. We then demonstrate the applications of COVID-19 transmission data to model the spread of the real-world disease. The impacts of physical distancing and personal protection equipment are also discussed in relevance to the COVID-19 spread. We compare our results on physical distancing effects to other methods such as the SEIR (Susceptible-Exposed-Infected-Recovered) model and the SEIRS (Susceptible-Exposed-Infected-Recovered-Susceptible) model.

Recent Advances in Computational PDEs for Finance 1

Organizer: **Christina Christara**

A high order method for pricing of financial derivatives using radial basis function generated finite differences

Lina von Sydow

Department of Information Technology, Uppsala Universitet, Sweden

We consider the numerical pricing of financial derivatives using Radial Basis Function generated Finite Differences in space. Such discretization methods have the advantage of not requiring Cartesian grids. Instead, the nodes can be placed with higher density in areas where there is a need for higher accuracy. Still, the discretization matrix is fairly sparse. As a model problem, we consider the pricing of European options in 2D. Since such options have a discontinuity in the first derivative of the payoff function which prohibits high order convergence, we smooth this function using an established technique for Cartesian grids. Numerical experiments show that we acquire a fourth order scheme in space, both for the uniform and the nonuniform node layouts that we use. The high order method with the nonuniform node layout achieves very high accuracy with relatively few nodes. This renders the potential for solving pricing problems in higher spatial dimensions since the computational memory and time demand become much smaller with this method compared to standard techniques.

Operator splitting schemes for option valuation under the two-asset Merton jump-diffusion model

Karel In 't Hout

Department of Mathematics, University of Antwerpen, Belgium

Under the two-asset Merton jump-diffusion model, the value of a European-style option satisfies a two-dimensional time-dependent partial integro-differential equation (PIDE) and the value of an American-style option satisfies a two-dimensional time-dependent partial integro-differential complementarity problem (PIDCP). We study a variety of recent and novel operator splitting schemes when applied to these problems, with a keen focus on implicit-explicit (IMEX) and alternating direction implicit (ADI) methods. Each of these schemes conveniently treats the nonlocal integral part in an explicit fashion. Through ample numerical experiments we investigate the convergence behaviour of the various splitting schemes and study their relative performance.

This research is joint work with Lynn Boen.

A fitted multi-point flux approximation method for pricing two-asset options

Rock Stephane Koffi

Department of Mathematics, University of Cape Town, South Africa

In this work, we develop novel numerical methods based on the multi-point flux approximation (MPFA) method to solve the degenerated partial differential equation (PDE) arising from pricing two-asset options. The standard MPFA is used as our first method and is coupled with a fitted finite volume in our second

method to handle the degeneracy of the PDE and the corresponding scheme is called fitted MPFA method. The convection part is discretized using the upwinding methods (first and second order) that we have derived on non-uniform grids. The time discretization is performed with θ-Euler methods. Numerical simulations show that our new schemes can be more accurate than the current fitted finite volume method proposed in the literature.

Comparison of numerical PDE and asymptotic approaches for stochastic default intensity in bilateral XVA pricing

Yuwei Chen

Department of Computer Science, University of Toronto, Canada

Adjusting derivative prices to take into account default risk has attracted the attention of several researchers and practitioners, especially after the 2007-2008 financial crisis. We derive a novel partial differential equation (PDE) model for derivative pricing including the adjustment for default risk, assuming that the default risk of one of the counterparties (the buyer) follows a Cox-Ingersoll-Ross (CIR) process, while the other party has constant default risk. The time-dependent PDE derived is of Black-Scholes type and involves two "space" variables, namely the asset price and the buyer default intensity, as well as a nonlinear source term. We formulate boundary conditions appropriate for the default intensity variable. The numerical solution of the PDE is based on standard finite differences, and a penalty-like iteration for handling the nonlinearity. Using singular perturbation theory, we also develop a novel asymptotic solution formula for the adjusted price of derivatives. We present numerical results that indicate stable second order convergence for the 2D PDE solution in terms of the discretization size. We compare the effectiveness of the 2D PDE and asymptotic solutions. We study the effect of various numerical and market parameters to the values of the adjusted prices and to the accuracy of the computed solutions.

Numerical methods in muscle modelling and its applications 2

Organizer: **Sebastian Dominguez, Raymond Spiteri**

From skeletal to cardiac muscle modelling and vice versa

Sebastian Dominguez

Department of Mathematics and Statistics, University of Saskatchewan

The study of the behaviour of muscle tissues has come to be of major interest in the context of diseases or conditions. Numerical simulations are particularly important and useful in order to help researchers to obtain important conclusions without the need of in-person laboratory tests. In this talk we walk through some developments regarding numerical methods and some applications in computational biomechanics. These methods are used to resolve the mechanics and the electrophysiological details of skeletal and cardiac muscle, and some applications where these numerical methods are of great help. We focus on a mechanical model describing the deformations of skeletal muscle, and on electrophysiological models describing the diffusion of the electric potential in cardiac muscle. We include details on a 3D continuum model that describes the deformation of skeletal muscle, the well known monodomain and bidomain models, as well as the newly developed EMI model. The results presented here are a joint work with R. Spiteri (USask), K.

Green (USask), J. Reimer (USask), N. Nigam (SFU), J. Wakeling (SFU), S. Ross (SFU), D. Ryan (SFU), and B. Borsterlee (NeuRA).

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Skeletal muscle: modeling and simulation of isometric contractions

Nilima Nigam

Department of Mathematics, Simon Fraser University, Canada

In this work we present a 3-D fibre-reinforced continuum model of skeletal muscle, and discuss the highly nonlinear system which arises even in the setting of quasistatic deformations. We describe the features of skeletal which are encoded in our model - including the capability to support distinct tissues, fibre types, and fat infiltration, and a finite element discretization for the system. A key challenge has been to fit model parameters to experimental data. Computational experiments (conducted within the deal.ii finite element library) lead to fascinating emergent behaviours, which in turn have important physiological implications. This is part of an ongoing collaboration with James Wakeling, Sebastian Dominguez, Stephanie Ross, Ryan Konno and Hadi Rahemi.

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An interdisciplinary approach to understanding the contractile consequences of muscle tissue mass

Stephanie Ross

Department of Biomedical Physiology and Kinesiology, Simon Fraser University, Canada

Skeletal muscles are the motors that drive human and animal locomotion. Yet despite their fundamental importance, our understanding of whole muscle behaviour is relatively limited due to practical and ethical considerations that hinder accurate in vivo measures. To estimate the behaviour of whole muscles, measures of single fibres or fibre bundles are often extrapolated to larger sizes without considering or accounting for the greater muscle mass. In this research, we used complementary measures of muscle in living animals and novel 1D phenomenological and 3D continuum muscle models to determine the effects of muscle mass on the contractile performance of whole skeletal muscle. In the first study, we used a damped harmonic oscillator in series with the 1D muscle model examine the effects of distributed muscle mass on mass- specific mechanical work per cycle during cyclic contractions. We found that when the mass- enhanced muscle model was isometrically scaled from the size of a fibre bundle up to a whole human plantarflexor muscle, the mass-specific work per cycle decreased. In the second study, we examined the effects of muscle mass on the contractile behaviour of in situ rat plantaris muscle to validate the 1D muscle model. In the third study, we simulated cyclic contractions of a fully dynamic 3D continuum muscle model that accounts for tissue mass effects across a range of muscle sizes. We additionally compared the effects of greater muscle mass on tissue accelerations of the 3D muscle model to that of the in situ rat plantaris muscle from the second study to qualitatively validate the model simulations. We found that increasing the mass of the 3D muscle increased its volume-specific kinetic energy and was associated with lower mass- specific mechanical work per cycle. In our fourth study, we examined the effects of muscle mass on the metabolic cost and efficiency of muscle during cyclic contractions and how tendons of different stiffnesses alter these relationships. We found that larger muscles with greater mass are less efficient, primarily due to lower mass-specific mechanical work, and that the work and efficiency penalty of larger muscles can be offset to a certain extent by a tendon of optimal stiffness. Taken together, the results of these studies highlight that muscle mass is an important determinant of whole skeletal muscle behaviour.

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Modelling the multiscale phenomena of diseased skeletal muscle tissue

Ryan Konno

Department of Mathematics, Simon Fraser University

Skeletal muscle structure and the changes that occur in diseased muscle tissue cross several physical length scales. Diseased muscle tissue can have alterations to the individual contractile components inside the muscle fibres and to the extracellular matrix that surrounds these fibres. Cerebral palsy is one such permanent disorder that results in substantial changes to the skeletal muscle microstructure. A fundamental component to muscle function is the sarcomere, which produces both active and passive forces. During cerebral palsy, the sarcomeres are typically lengthened, which results in increased passive force and decreased active force. Additionally, there is often an observed increase in the volume fraction of the extracellular matrix, which has a large contribution to the overall muscle stiffness. However, it is difficult using experimental techniques to determine the effect of the individual microscopic components on the overall muscle mechanics, and so a modelling approach is required. We use a 3D continuum model for muscle to investigate the behaviour of muscle in response to cerebral palsy, and determine the component of muscle that has the most substantial effect on skeletal muscle mechanics.

Young Canadian Researchers – Contributions to Mathematical Modelling in Public Policy 2

Organizer: **Monica Cojocaru, Zahra Mohammadi, Darren Flynn-Primrose**

Mathematical modelling to inform Ontario's COVID-19 response: successes, challenges, and lessons learned

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The McMaster University Theoretical Biology lab has been making COVID-19 forecasts for several jurisdictions around the world through- out the pandemic. We have developed a compartmental epidemiological model for COVID-19, as well as the publicly-available McMaster- Pandemic R package that performs statistical fits of the model to dis- ease data. These fits are used to estimate key epidemiological metrics and to generate short-term forecasts of disease spread under various intervention scenarios, all with the goal of informing public health pol- icy. In this talk, I will present the McMasterPandemic model, and focus on the COVID-19 forecasts our group has been making for the province of Ontario. These projections are provided to the Ontario Modelling Consensus Table, and are used in conjunction with forecasts from other research groups to brief the Health Coordination Table of the Ontario Ministry of Health, as well as the public in semi-monthly press conferences.

I will reflect on our experiences in trying to use mathematical models to inform public policy over the course of an unfolding pandemic, out- lining our group?s successes, the challenges we?ve encountered, and the lessons we have learned along the way.

Mobility during the pandemic and its markers of disease spread

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The outbreak of Coronavirus disease 2019 (COVID-19) originated in Wuhan, China, has affected the lives of millions of people globally. Throughout the last year, the reproduction number of COVID-19 is widely used by decision-makers to explain their strategies to control the COVID-19 pandemic. In this work, we compare the effective re- production numbers from real incidence data with theoretical estimates for 12 regions/countries from February 2020 to January 2021. We con- sider mobility reductions, behavioral activity as contact rate, and other nonpharmaceutical interventions(NPIs) in each region to get more accurate effective reproduction numbers in this time interval. In each region, the use of and adherence to NPIs measures, principally social distancing and mask-wearing, had largely reached an equilibrium over summer and early fall of 2020. However, as throughout much of the rest of the Northern Hemisphere, the rate of transmission increased dramatically starting in July. Cellphone mobility data combined with contact rates allow us to investigate the effects of mobility reduction and other NPIs measures on decreasing the effective reproduction numbers to respond to the pandemic in the absence of vaccinations. We quantify this additional effect, which may be attributable to seasonality as seen in other respiratory diseases e.g. influenza, RSV, etc.

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Mathematical Modeling and Analysis of Human Gait

N. Yu

Department of Mathematics, Ryerson University, Canada

Walking is a basic activity most of us do every day. However unstable gait, even falling, could cause serious damages, especially for seniors. Approximately 1/3 of adults aged 65 years and older fall each year in Canada. This project is aimed to investigate the fundamental mechanisms of stable walking using mathematical models, numerical simulation, and experimental data of human gait.

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Cancer: 5-year survival vs. Network Statistics - From Correlation to Application

M.A.L. Croix, K. Wilkie

Department of Mathematics, Ryerson University, Canada

As computing power is increasingly applied to problems from biological science, our ability to generate data sometimes outpaces our ability to meaningfully interpret it. As an example, we look at an observation from cancer research. As per Breitkreutz et al. 2012*, the 5-year survival rate for various forms of cancer is negatively correlated with the degree-entropy of the protein-protein interaction networks associated with the cancer type. The 5-year survival rate is suggested as a proxy for treatability, while degree entropy is hypothesized to further correlate with some as yet unidentified biologically meaningful property, but in the absence of a causative mechanism, how can knowing about this correlation (or any of the related correlations appearing in subsequent literature) help us meaningfully influence health outcomes?

Any correlation can be used to suggest a set of axes against which to perform clustering, and search for outliers, but this kind of approach is prone to identifying reassuring, but unhelpful trends like: - research

spending improves cancer survival, - conveniently located tumors are easier to treat, and - early diagnosis leads to longer survival after diagnosis. In moving beyond these superficial observations, we face the obstacle that neither network statistics nor cancer survival rates are intrinsic properties. Both evolve, abeit separately, in response to the state of current knowledge. Our approach involves incorporating this time- dependence and then using data visualization to help contextualize the degree to which purported patterns do and do not exist.

Mathematical Modelling of COVID-19 Transmission and Mitigation Strategies: Efforts to End the Pandemic 2

Organizer: **Jude Kong, Elena Aruffo**

Studying social awareness of physical distancing in mitigating COVID-19 transmission

Xiaoying Wang

Department of Mathematics, Trent University, Canada

Since the initial identification of a COVID-19 case in Wuhan, China, the novel disease quickly becomes a global pandemic emergency. In this paper, we propose a dynamic model that incorporates individuals' behavior change in social interactions at different stages of the epidemics. We fit our model to the data in Ontario, Canada and calculate the effective reproduction number within each stage. Results show that ¿1 if the public's awareness to practice physical distancing is relatively low and ¡1 otherwise. Simulations show that a reduced contact rate between the susceptible and asymptomatic/unreported symptomatic individuals is effective in mitigating the disease spread. Moreover, sensitivity analysis indicates that an increasing contact rate may lead to a second wave of disease outbreak. We also investigate the effectiveness of disease intervention strategies. Simulations demonstrate that enlarging the testing capacity and motivating infected individuals to test for an early diagnosis may facilitate mitigating the disease spread in a relatively short time. Results also indicate a significantly faster decline of confirmed positive cases if individuals practice strict physical distancing even if restricted measures are lifted.

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Modeling mitigation strategies to contain COVID-19

Lauren Childs

Department of Mathematics, Virginia Tech, USA

Voluntary individual quarantine and voluntary active monitoring of contacts are core disease control strategies for emerging infectious diseases such as COVID-19. Given the impact of quarantine on resources and individual liberty, it is vital to assess under what conditions individual quarantine can more effectively control COVID-19 than active monitoring. To estimate the comparative efficacy of individual quarantine and active monitoring of contacts, we fit a stochastic branching model to reported parameters for the dynamics of the disease. Specifically, we fit a model to the incubation period distribution and to two estimates of the serial interval distribution: a shorter one with a mean serial interval of 4.8 days and a longer one with a mean of 7.5 days. To assess variability in the availability of resources, we considered two feasibility settings: high-feasibility with 90% of contacts traced, a half-day average delay in tracing and symptom recognition, and 90% effective isolation; and low-feasibility with 50% of contacts traced, a 2-day average

delay, and 50% effective isolation. Model fitting by sequential Monte Carlo resulted in a mean time of infectiousness onset before symptom onset for the longer serial interval of 0.51 days. Individual quarantine in high-feasibility settings, where at least 75% of infected contacts are individually quarantined, contains an outbreak of SARS-CoV-2 with a short serial interval 84% of the time. However, in settings where the outbreak continues to grow (e.g., low-feasibility settings), so too will the burden of the number of contacts traced for active monitoring or quarantine, particularly uninfected contacts (who never develop symptoms). Our model highlights the urgent need to consider data-driven policy decisions regarding the cost?benefit comparisons of individual quarantine versus active monitoring of contacts. As an epidemic grows, it is important to consider when these interventions are no longer feasible and broader mitigation measures must be implemented. To the extent that individual quarantine and active monitoring can be performed, they can help mitigate the spread of SARS-CoV-2.

Combining data forecasting with scenario-based modeling for insights into a rapidly changing outbreak situation

Matt Betti

Department of Mathematics, Mount Allison University, Canada

We present a simple, modified SIR model with the intended use of bridging the gap betweeen data-fitted forcasts and modeled scenario-based forecasting. Using a combination of data-driven forecasting, simple model structures, and ensemble fitting we are able to determine mid-range predictions for rapidly changing situations. Using results over the past year on COVID-19 we will highlight the strengths of such an approach when it comes to forecasting trajectories and how this can be used to help policy and decision making.

Recent Advances in Computational PDEs for Finance 2

Organizer: **Christina Christara**

Numerical solution of a PDE model for the pricing of renewable energy certificates

Carlos Vázquez Cendón

Department of Mathematics, University of A Coruña, Spain

Among the policies followed by countries to promote the investment in renewable energies, the use of Renewable Energy Certificates or RECs (also referred as Green Certificates or GCs in Europe) has been incorporated. When renewable energy generators achieve certain criteria, they receive one certificate for a specific unit of renewable electricity produced. Many countries have developed markets where RECs are traded. In this work, we pose a new PDE model for the pricing of RECs, which mainly includes a semilinear equation in two spatial variables, which represent the generation rate and the accumulation of green certificates. More precisely, the semilinear PDE includes the typical degenerate diffusion term (as in Asian options) and a nonlinearity in the first order derivatives, which can be formulated in terms of a maximal monotone operator. Appropriate numerical methods for the nonlinear term and the full discretization are proposed. Thus, semi-Lagrangian methods are proposed for the time discretization while finite differences or finite elements can be used for the spatial discretization. Additionally, a duality method is proposed for the nonlinearity associated to the first order derivatives. An academic and a real case are solved to illustrate the performance of the model and the numerical methods.

Joint work with María Baamonde (University of A Coruña), M. Carmen Calvo-Garrido (University of A Coruña) and Michael Coulon (University of Sussex).

Tree-based approaches to solve BSDEs with applications in finance

Long Teng

Applied Mathematics / Numerical Analysis (AMNA), Bergische Universität Wuppertal, Germany

In this work, we study solving backward stochastic differential equations (BSDEs) numerically using the regression trees. Based on the general theta-discretization for the time-integrands, we show how to efficiently use regression tree-based methods to solve the resulting conditional expectations. Several numerical experiments including high-dimensional problems are provided to demonstrate the accuracy and performance of the tree-based approach. For the applicability of BSDEs in financial problems, we apply our tree-based approach to the Heston stochastic volatility model, and an European financial derivative with different interest rates for borrowing and lending.

Recurrent Pricing Network for Computing Multi-Asset American Option and Delta Hedging Parameters

Justin Wan

Cheriton School of Computer Science, University of Waterloo, Canada

In this talk, we propose a recurrent neural network (RNN) approach for pricing American option with many assets as well as computing the deltas for hedging for the entire time and spatial domain. The existing neural network models require either large feedforward networks or a sequence of neural networks in order to capture the time dynamics. The RNN approach takes advantage of the "recurrent" property that mimics time stepping in solving the American option PDE. In particular, we will explore the Long-Short Term Memory (LSTM) and Gated Recurrent Unit (GRU) model in our option pricing framework. In addition, we will adopt the backward stochastic differential equation (BSDE) formulation for American option so that we can apply Monte-Carlo method for solving high dimensional PDEs. The computational cost is linear in d and N, where d is the dimension and N is the number of time steps. This is in contrast with other existing methods which are quadratic in both d and N. We will demonstrate the efficiency of our model by numerical examples of different multi-asset American option problems, and how it compares with the state-of-the-art approaches.

Penalty Methods for Nonlinear HJB PDEs

Ruining (Ray) Wu

Department of Computer Science, University of Toronto, Canada

There are numerous financial problems that are naturally posed as optimal control problems, leading to HJB or HJBI equations. We reformulate these problems as nonlinear PDEs and suggest efficient numerical methods for handling the nonlinearity in the PDE through an adaptation of the discrete penalty method. We formulate a penalty-like method for the case with European exercise rights, and extend this to American

exercise rights resulting in a double penalty method. Compared with previous work, our method is more general as it is able to handle nonlinearity in the derivative terms (Delta and Gamma). We also use our findings to improve the policy iteration algorithms that our algorithms are based off of. In both the cases of European and American exercise rights, the improved policy iteration algorithm is shown to be equivalent to the penalty one. Numerical results are provided showing clear second-order convergence, and where applicable, we prove the convergence of our algorithms.

Mathematical Advances in Batteries 1

Organizer: **Iain Moyles, Matthew Hennessy**

Mathematical Modelling of Lithium-ion batteries on the nanoscale

Laura Keane

York University, Canada

Recent advances in electrode chemistry have allowed for cylindrical nanowire geometries exhibiting low capacity fade. However, the performance of these electrodes are very sensitive to experimental conditions and early charge behaviour and thus it is important to understand the lithium transport process in these systems. We introduce a mathematical model for lithium transport in a nanowire electrode with a solid state electrolyte. We simulate discharge and concentration dynamics and compare to experimental results.

Fast Simulations of Lithium-Ion Battery Degradation

Valentin Sulzer

University of Michigan, USA

We propose an algorithm to speed up physics-based battery lifetime simulations by one to two orders of magnitude compared to the state-of-the-art. This algorithm makes use of the difference between the ?fast? timescale of battery cycling and the ?slow? timescale of battery degradation by adaptively selecting and simulating representative cycles, and hence requires fewer cycle simulations to simulate the entire lifetime. This enables interactions with the simulations on a human timescale [1], and therefore opens the possibility for much faster and more accurate model development, testing, and comparison with experimental data.

Physics-based electrochemical models, based on porous electrode theory [2], are very useful for understanding battery degradation, and hence predicting lifetime, since they can directly simulate a wide range of degradation mechanisms at various scales. Many modeling studies investigate the degradation for a single cycle, and there have been significant advances in making simulations of individual cycles as efficient as possible [3,4,5]. However, relatively few simulations of the entire battery life have been conducted. This may be due to the complexity of these models, both in terms of implementation effort and computational time. Previous work has addressed the implementation challenges [6], and this work addresses the computational time.

Our proposed multiple scale algorithm simulates degradation over the entire lifetime of a battery in just a few seconds. The algorithm is implemented in the open-source battery modeling package PyBaMM [6] and thus can easily be used to simulate any (current or future) aging model implemented there. Alternatively, it can easily be incorporated in other simulation frameworks. We demonstrate the algorithm in a few case studies, including degradation mechanisms such as SEI formation, lithium plating, and loss of active

material. In each case we achieve one to two order of magnitude speed-ups compared to the baseline. Since the speed-up combines multiplicatively with speed-ups in simulation of a single cycle, the entire lifetime of the battery can be simulated in just a few seconds.

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A fast solver for Li-ion thermal P2D model

Rachel Han

University of British Columbia, Canada

A pseudo-two-dimensional (P2D) model is a complex mathematical model that can capture the electrochemical process in Li-ion batteries. However, the model also brings a heavy computational burden. We present a method for fast computation of the thermal P2D model which must be used when the simplifications are not accurate enough. We also employ automatic differentiation, using an open source package named JAX, for robustness. The method alleviates the computational bottleneck inherent in P2D models without compromising accuracy.

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On Uncertainty Quantification in the Parametrization of Newman-type Models of Lithium-ion Batteries

Bartek Protas

McMaster University, Canada

We consider the problem of parameterizing Newman-type models of Li-ion batteries focusing on quantifying the inherent uncertainty of this process and its dependence on the discharge rate. In order to rule out genuine experimental error and instead isolate the intrinsic uncertainty of model fitting, we concentrate on an idealized setting where "synthetic" measurements in the form of voltage curves are manufactured using the full, and most accurate, Newman model with parameter values considered "true", whereas parameterization is performed using simplified versions of the model, namely, the single-particle model and its recently proposed corrected version. By framing the problem in this way, we are able to eliminate aspects which

affect uncertainty, but are hard to quantity such as, e.g., experimental errors. The parameterization is performed by formulating an inverse problem which is solved using a state-of-the-art Bayesian approach in which the parameters to be inferred are represented in terms of suitable probability distributions; this allows us to assess the uncertainty of their reconstruction. The key finding is that while at slow discharge rates the voltage curves can be reconstructed quite accurately, this can be achieved with some parameter varying by 300% or more, thus providing evidence for very high uncertainty of the parameter inference process. As the discharge rate increases, the reconstruction uncertainty is reduced but at the same time the fits to the voltage curves becomes less accurate. These observations highlight the ill-posedness of the inverse problem of parameter reconstruction in models of Li-ion battery operation. In practice, using simplified models appears to be a viable and useful strategy provided that the assumptions facilitating the model simplification are truly valid for the battery operating regimes in which the data was collected. [joint work with Jose Morales Escalante, Smita Sahu and Jamie M. Foster]

Novel and Unconventional Reaction–Diffusion Problems 1

Organizer: **Yana Nec, Justin Tzou**

Oscillating spots in reaction-diffusion systems

Shuangquan Xie

Department of Mathematics and Statistics, Dalhousie University, Canada

In this talk, I will discuss a three-component Schnakenberg model, whose key feature is that it has a solution consisting of N spots that undergoes Hopf bifurcations concerning N distinct modes nearly simultaneously. This induces complex oscillatory dynamics of the spikes, not seen in typical two-component models. We find that the long-time behavior of a two-spike solution beyond Hopf bifurcation can be either in-phase or out-of-phase oscillations.Both in and out of phase oscillations are stable, coexist for the same parameter values, and the fate of motion depends solely on the initial conditions. For a general N-spot solution, we show that there are only two stable oscillatory states even though N Hopf modes become unstable. The oscillatory state we can observe is determined by the initial perturbation.

Differential equation model for central-place foragers with memory: implications for bumble bee crop pollination

Pau Capera-Aragones, Eric Foxal, Rebecca C. Tyson

Department of Computer Science, Mathematics, Physics and Statistics, University of British Columbia Okanagan, Canada

Bumble bees provide valuable pollination services to crops around the world. However, their populations are declining in intensively farmed landscapes. Understanding the dispersal behaviour of these bees is a key step in determining how agricultural landscapes can best be enhanced for bumble bee survival. In our work we develop a partial integro-differential equation model to predict the spatial distribution of foraging bumble bees in dynamic heterogeneous landscapes. In our model, the foraging population is divided into two subpopulations, one engaged in an intensive search mode (modeled by diffusion) and the other engaged in an extensive search mode (modeled by advection). Our model considers the effects of resource-dependent switching rates between movement modes, resource depletion, central-place foraging behaviour, and memory.

We use our model to investigate how crop pollination services are affected by wildflower enhancements. We find that planting wildflowers adjacent to a crop can increase the pollination services to the crop, and we quantify this benefit as a function of the location, quantity, and quality of the planted wildflowers.

Non-hexagonal lattice minimizers in interacting systems

Juncheng Wei

Department of Mathematics, University of British Columbia, Canada

In this talk I will discuss optimal lattices in two interacting systems. In the first system, a two species interacting system motivated by the density functional theory for triblock copolymers contains long range interaction that affects the two species differently. In a two species periodic assembly of discs, the two species appear alternately on a lattice. The minimal two species periodic assembly is the one with the least energy per lattice cell area. There is a parameter b in [0, 1] and the type of the lattice associated with the minimal assembly varies depending on b. We show that there are several thresholds defined by a number B = 0.1867... If b ? [0, B), the minimal assembly is associated with a rectangular lattice; if b ? [B, 1?B], the minimal assembly is associated with a square lattice; if b ? (1?B, 1], the minimal assembly is associated with a rhombic lattice. Only when b = 1, this rhombic lattice is the hexagonal lattice. None of the other values of b yields the hexagonal lattice, a sharp contrast to the situation for one species interacting systems, where the hexagonal lattice is ubiquitously observed. In the second system, we consider the lattice arrangements of vortices in competing systems of Bose-Einstein condensates as derived and conjectured (and numerically and experimentally verified) by Mueller-Ho. This becomes minimizing the sum of two Theta functions. We rigorously establish the optimality of non-hexagonal patterns which partially solve the Muller-Ho Conjecture.

Investigating the impact of the mycorrhizal inoculum on the resident fungal community and on plant growth

Maria M. Martignoni, Jimmy Garnier, Miranda M. Hart, **Rebecca Tyson**

Department of Computer Science, Mathematics, Physics and Statistics, University of British Columbia Okanagan, Canada

In the last few decades, microbial inoculants have been used as organic fertilizers worldwide. Among the most widely used commercial products are arbuscular mycorrhizal (AM) fungi, as these fungi can associate with a variety of crops. Despite the potential benefits for soil quality and crop yield associated with AM fungal colonization, experiments assessing the persistence of the fungi in the field have yielded inconsistent results. Additionally, it is not yet clear whether or not the introduction of commercial inoculants could lead to changes to the resident fungal community, and eventually to invasion of the commercial products with a possible displacement of resident species. Here we use a partial differential equation model to assess the potential biodiversity risks and productivity benefits deriving from inoculation. We study the impact of AM fungal inoculation on the resident fungal community and on plant growth at a landscape scale. We determine how inoculant persistence and spread are affected by its competition with resident fungal species, by its mutualist quality, and by fungal dispersal. Our findings suggest that the increase in fungal abundance due to inoculation always leads to a short-term increase in host productivity, regardless of inoculant identity. However, the use of strongly competing inoculants constitutes a biodiversity risk, and may result in the invasion of low quality mutualists.

Utilizing AI and Machine Learning Techniques for Data Analytics 1

Organizer: **Wenying Feng, Jimmy Huang, Jianhong Wu**

QoS prediction – new strategy with clustering and tensor decomposition

Sheng Chai

School of Computing, Queen's University, Canada

Web service recommendation based on Quality of Service (QoS) value has been widely researched. At present, most of the existing methods adopt the idea of collaborative filtering for web service QoS prediction, aiming to provide service recommendations and improve the accuracy of prediction results. The collaborative filtering algorithm generally uses feedback data from some of the neighbors for collaborative prediction, and the prediction results are still not very satisfactory when the user-service-time QoS data is sparse. Especially in the face of the increase of new users, the prediction results about new users will worsen. We address the problem that hinders the further development of web services technology in practical applications. A two-step strategy approach is proposed, which includes K-means clustering and tensor decomposition methods. First, a preprocessing process based on K-means clustering was designed to cluster the initial data in the hope of discovering the implicit relationships between the data. In the second step, the clustered data objects are used as input and applied to the tensor decomposition method to complete the QoS prediction. Experimental results on the relevant dataset show the improvement in the web service recommendation.

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Challenging musical sub-genre classification using audio features

Miria Feng

Stanford University, USA

We evaluate two deep learning models which integrate convolutional and recurrent neural networks. We implement both sequential and parallel architectures for fine-grain musical subgenre classification. Due to the exceptionally low signal to noise ratio (SNR) of our low level mel-spectrogram dataset, more sensitive yet robust learning models are required to generate meaningful results. We investigate the effects of three commonly applied optimizers, dropout, batch regularization, and sensitivity to varying initialization distributions. The results demonstrate that the sequential model specifically requires the RMSprop optimizer, while the parallel model implemented with the Adam optimizer yielded encouraging and stable results achieving an average F1 score of 0.63. When all factors are considered, the optimized hybrid parallel model outperformed the sequential in classification accuracy and system stability.

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Affective response generation with transformer

Lei Liu

York University, Canada

Similar to the interpersonal communications, affect and emotion play critical roles in human-machine conversations. To conduct chatbots that generate diverse responses with rich affects and emotions, extensive researches on modelling and incorporating affective information or emotion categories into dialogue systems

has been done. However, these work was typically built on top of the recurrent neural network (RNN) based sequence-to-sequence model which tends to generate short responses with less affects. Since Transformer performs better than RNN in several language generation tasks, we take the advantage of it and propose a Transformer-based affective response generation model that can generate longer and relevant responses with rich affects and appropriate semantics. Specifically, we propose to use affective embeddings as inputs to the Transformer model where both the affective information of the word and the semantics resided in its context can be embedded in the word representations; then, we propose Affective Scaled Dot-product Attention to selectively attend both the semantics and implicit affects in words; on top of it, we further present our Affective Multi-head Attention and accordingly propose to use it in three different approaches namely Affective Multi-head Self-attention, Affective Multi-head Encoder-decoder Attention and Masked Affective Multi-head Self-attention. We will compare responses generated by our models with that of baselines to demonstrate the effectiveness of our methods.

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Deep learning and applied math – how they might connect

Charles Ling

Department of Computer Science, Western University, Canada

The problems that deep learning and applied math are solving seem different (as far as I can tell). In this talk, I will discuss several recent progress in deep learning that could solve some applied math problems. I hope my talk can connect the two fields so they can benefit each other in the future.

Statistical and Epidemiological Modelling of COVID-19

Organizer: **Andy Wan, Samuel Wong**

Statistical challenges in the analysis of sequence and structure data for the COVID-19 spike protein

Shiyu He

Department of Statistics and Actuarial Science, University of Waterloo, Canada

As the major target of many vaccines and neutralizing antibodies against SARS-CoV-2, the spike (S) protein is observed to mutate over time. In this paper, we present statistical approaches to tackle some challenges associated with the analysis of S-protein data. We build a Bayesian hierarchical model to study the temporal and spatial evolution of S-protein sequences, after grouping the sequences into representative clusters. We then apply sampling methods to investigate possible changes to the S-protein?s 3-D structure as a result of commonly observed mutations. While the increasing spread of D614G variants has been noted in other research, our results also show that the co-occurring mutations of D614G together with S477N or A222V may spread even more rapidly, as quantified by our model estimates.

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Networks of necessity: simulating strategies for COVID-19 mitigation among disabled people and their caregivers

Michael Lindstrom

Department of Mathematics, University of California Los Angeles, USA

To slow the spread of COVID-19, many countries initially implemented interventions against the disease, such as limiting contacts and mask-wearing. However, approximately 7% of Canadians have a disability requiring assistance from home care aides to assist with activities of daily living and thus contact-limiting applies differently to these groups. In this talk, we look into an agent-based network model of COVID-19 and the effects of various interventions upon the disabled and care aide communities of Ottawa. Our model accounts for multiple disease compartments, including allowing for asymptomatic transmission; different types of contacts and associated risks; and different contact distributions based on an individual's occupation. Our work suggests that care aides and disabled people are strongly affected by global intervention strategies and that care aides may be one of the most influential groups in spreading the illness.

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Conformational variability of loops in the SARS-CoV-2 spike protein

Zongjun Liu

Department of Mathematics and Statistics, Queen's University, Canada

The SARS-CoV-2 spike (S) protein facilitates viral infection, and has been the focus of many structure determination efforts. This paper studies the conformations of loops in the S protein based on the available Protein Data Bank (PDB) structures. Loops, as flexible regions of the protein, are known to be involved in binding and can adopt multiple conformations. We identify the loop regions of the S protein, and examine their structural variability across the PDB. While most loops had essentially one stable conformation, 17 of 44 loop regions were observed to be structurally variable with multiple substantively distinct conformations. Loop modeling methods were then applied to the S protein loop targets, and loops with multiple conformations were found to be more challenging for the methods to predict accurately. Sequence variants and the up/down structural states of the receptor binding domain were also considered in the analysis.

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Assessing the effectiveness of regional physical distancing measures of COVID-19 in rural regions of British Columbia

Geoffrey McGregor

Department of Mathematics and Statistics, University of Northern British Columbia, Canada

Early epidemiological modelling of the transmission of COVID-19 within British Columbia (BC), Canada, mainly focused on provincial-wide prediction using data from populated regions. While this rapid modelling effort was instrumental at the time on assessing the effectiveness of physical distancing measures, the provincial-wide model did not take into account for regional differences, such as in population density and testing availability in rural regions. We present a regionalized version of an epidemiological model introduced in [Anderson et al, 2020] to study the impacts of regionalized modelling throughout BC between March and December 2020. In particular, we study the effects of physical distancing measures for the spread of COVID-19 in regional areas within BC, using the reported cases of the five provincial Health Authorities. Utilizing a hierarchical Bayesian model with time-varying regional parameters to account for the relative reduction in contact due to physical distancing and increased testing, we examine the differences in regionalized basic reproduction number, modelled prevalence, fraction of normal contacts and proportion of anticipated cases.

In this talk, a detailed overview of the regionalized model will be presented, along with results highlighting the significant differences observed between the provincial-wide and regional models.

This is joint work with Jennifer Tippett (UNBC), Andy Wan (UNBC), Mengxiao Wang (UWaterloo) and Samuel Wong (UWaterloo).

Mathematical Advances in Batteries 2

Organizer: **Iain Moyles, Matthew Hennessy**

Asymptotic methods for the estimation of lithium transport properties in lithium-ion batteries

Ferran Brosa Planella

WMG, University of Warwick, United Kingdom

Model parameterisation is a crucial point to obtain accurate quantitative predictions and can be a very challenging task, especially in models with a large number of parameters such as battery models. Given that estimating all the parameters from a single experimental setup is usually not feasible, different sets of experiments have been developed for this task.

One of the key phenomena that determines the behaviour of lithium-ion batteries is the lithium transport in the electrodes. This transport is usually modelled as a Fickian diffusion process with a concentration dependant diffusivity, and the methods to determine the diffusivity have been used for decades. However, these methods are not specific for porous electrode batteries and thus this can lead to confusion and inconsistency when using the parameters obtained by this method in the battery models. We present a new approach to characterise the lithium transport properties in lithium-ion battery models, using reduced models obtained by asymptotic methods. The asymptotic methods ensure that the reduced model used in the parameterisation is consistent with the full model and highlight the limitations of the approach, so its range of application is clear. Because this approach is systematic, it also sets the grounds to parameterise more complex transport models using the same experimental setup.

Mechanical deformations in lithium-ion batteries

Jamie Foster

School of Mathematics & Physics, University of Portsmouth, United Kingdom

I will present some work in progress on modelling the mechanical deformations that occur during electrode manufacture (calendaring) as well as during electrochemical cycling. Relatively little modelling has been done concerning the mechanics of lithium-ion batteries, but it is important to develop an understanding because mechanical stresses/strains exacerbate device ageing thereby limiting their lifetime. A continuum modelling approach is taken in which the stresses/strains in the binder, active material and electrolyte are predicted as a result of external loading, and particle and binder swelling. Two models are presented: The first is relatively simple, and can be subjected to asymptotic homogenisation to yield a readily soluble multiscale model. The second is more complex, and is more expensive to solve but is better capable of treating large stress/strain scenarios in which nonlinear responses are important.

Identifiability and parameter estimation of a lithium-ion battery model using nonlinear impedance spectroscopy

Toby Kirk

Mathematical Institute, University of Oxford, United Kingdom

Electrochemical impedance spectroscopy (EIS) is a widely-used non-invasive technique to investigate lithium-ion batteries and determine model parameters. It corresponds to the application of a small amplitude sinusoidal current of a single frequency and measuring the linear (sinusoid of the same frequency) voltage response. As nonlinearities are neglected, some parameters are difficult or impossible to determine. Applying larger amplitude currents (nonlinear EIS) induces a nonlinear response, whereby the voltage contains higher frequency harmonics. We consider nonlinear EIS applied to a single-particle Li-ion battery model, and derive analytical expressions for these higher harmonics via an amplitude expansion. The signatures of the model nonlinearities within these harmonics are explored, and improvements to parameter estimation, relative to traditional EIS, is demonstrated using synthetic data.

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Reduced-order models of spirally-wound cells via homogenization

Robert Timms

Mathematical Institute, University of Oxford, United Kingdom

Numerical simulation of the electrochemical-thermal behaviour of cylindrical cells can pose a significant computational challenge. One approach is to directly solve the governing equations on the complicated spiral geometry, but this typically requires a large number of mesh elements and is computationally expensive. A more common approach is to ?unwind? the cell and solve an electrochemical problem along the length of the current collectors coupled to a 3D thermal problem on a cylindrical domain. While this approach reduces the computational burden, coupling the two problems together is no trivial task. In this talk, we discuss how asymptotic homogenization can be used to systematically derive reduced- order macroscopic models of conductive behaviour in spirally-wound layered materials in which the layers have very different conductivities. The analysis identifies three distinguished limits, which correspond to conventional homogenization, in which there is an effective diffusion coefficient, a novel limit of radial diffusion, and a so-called ?two-potential? limit. The two-potential limit is particularly novel, in that the solution exhibits interesting variations on the microscale, and the homogenized problem involves not one but two functions of the macroscale.

To demonstrate the effectiveness of the modelling approach to practical problems we provide comparisons between the solutions of the homogenized and full models using parameter values typical of an 18650-type cell.

Novel and Unconventional Reaction–Diffusion Problems 2

Organizer: **Yana Nec, Justin Tzou**

Analysis of scaling limits of the kinetic chemotaxis equations

Ryan Thiessen

University of Alberta, Canada

The kinetic chemotaxis equations have long been used to model biological processes. We will analyze a volume filling variant of the kinetic chemotaxis equations on the torus. Since the kinetic chemotaxis systems have well known blow-up solutions, we spend a considerable amount of time showing conditions for which solutions of the volume filling kinetic chemotaxis equations exist globally. Due to the individualist origins of the kinetic equation (velocity jump process), the system?s interesting population dynamics occur at a much larger space-time scale. Various approximation methods have been developed to explore these population dynamics, like the parabolic scaling and moment closures. In this thesis, we will explore these approximation methods in the context of chemotaxis, and we will prove two new results for the convergence of the scaling limits to the parabolic limit and the hyperbolic limit, respectively. In addition to the mathematical consequences of the approximation methods, we will delve into their underlying biological meaning, explain under what conditions the methods coincide, and discuss their differences. In developing these models, a few common features appear, such as anisotropic diffusion and chemotactic mixing. For the above macroscopic models, we develop a sophisticated numerical solver to investigate anisotropic pattern formation. To our surprise, we found new spatial criss-cross patterns due to competing cues, one direction given by anisotropy versus a different direction due to chemotaxis. A full analysis of these new patterns is not part of this thesis and is left for future work.

Boundary layer solutions in the singularly perturbed Gierer-Meinhardt model

Daniel Gomez, Linfeng Mei, Juncheng Wei

University of Pennsylvania, USA

The role of boundary conditions in pattern forming reaction-diffusion systems is often times neglected, with models typically assuming closed systems described by no-flux boundary conditions. A recent focus on bulk-surface coupled reaction-diffusion systems has highlighted the importance of inhomogeneous boundary conditions for intracellular pattern formation. In this talk, I will discuss recent work on the analysis of localized solutions arising in the singularly perturbed Gierer-Meinhardt model with inhomogeneous Neumann, Robin, and Dirichlet boundary conditions. In the case of a one-dimensional domain I will describe in detail how the inhomogeneities at the boundaries lead to the formation of stable asymmetric solutions. In higher-dimensional domains I will highlight recent results characterizing the existence and stability of certain boundary layer solutions.

Reaction-subdiffusion equations with linear reactions

Sean Lawley

Mathematics Department, University of Utah, USA

Deriving evolution equations accounting for both anomalous subdiffusion and reactions is notoriously difficult, even in the simplest cases. In contrast to normal diffusion, reaction kinetics cannot be incorporated into evolution equations modeling subdiffusion by merely adding reaction terms to the equations describing spatial movement. Various models of reaction-subdiffusion have been proposed, and the type of mesoscopic equation depends on subtle assumptions about the microscopic behavior of individual molecules. Furthermore, the correspondence between mesoscopic and microscopic models is not well understood. In this talk, we will introduce some reaction-subdiffusion models and describe recent results on their solution and stochastic representation.

Narrow escape problems in the elliptic domain and global optimization of locations of traps of different size

Jason Gilbert, Alexei Cheviakov

University of Saskatchewan, Canada

Narrow escape and narrow capture problems describing average times required for a randomly travelling Brownian particle to be trapped by a small trap or window have applications in various areas of science including cell biology, synaptic connections, species interaction in mathematical biology, and more. While for general domains, it is known how the escape time decreases with the increase of the trap sizes, for some specific 2D and 3D domains, higher-order asymptotic formulas have been established, providing the dependence of the escape time on the sizes and locations of the traps. Such results allow the use of global optimization to seek trap arrangements that minimize average mean first passage times (MFPT). In a recent paper by Iyaniwura, Wong, Macdonald and Ward, escape time expansion for a 2D near-disk and elliptic domain was derived, providing the dependence of the average MFPT on sizes and locations of small equal-sized internal traps. We generalize MFPT formulae to include the case of traps of different sizes, and compute optimal MFPT-minimizing trap arrangements for various trap numbers and sizes, and different domain eccentricities.

Utilizing AI and Machine Learning Techniques for Data Analytics 2

Organizer: **Wenying Feng, Jimmy Huang, Jianhong Wu**

Computing Structured Singular Values

Mutti-Ur Rehman

Department of Chemical Engineering, Massachusetts Institute of Technology, USA

A novel method for approximating structured singular values (also known as m-values) is proposed and investigated. These quantities constitute an important tool in the stability analysis of uncertain linear control systems as well as in structured eigenvalue perturbation theory. Our approach consists of an inner-outer iteration. In the outer iteration, a Newton method is used to adjust the perturbation level. The inner iteration solves a gradient system associated with an optimization problem on the manifold induced by the structure. Numerical results and comparison with the well known MATLAB function mussv, implemented in the MATLAB Control Toolbox, illustrate the behavior of the method.

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Influence of Geodemographic Factors on Power Consumption

Jitendar Singh

Trent University, Canada

The housing sector is a major consumer of electricity, and its demand will rise by 65 percent by the end of 2050. The electricity consumption of a home depends on various factors like house size, house type, employment, education, size of the family and family structure. However, the previous studies have only identified a limited number of social, economic, and dwelling factors. In our research, we explore the significance of 826 geodemographic factors. Geodemographics cover factors from a wide array of categories

like the economy, education, family, finance, housing, transport, health, and environment. We propose a methodology to study the correlation between the power consumption of a home and its geodemographic factors. We identify 354 factors that are highly significant. Then we examine the possibility of using geodemographic information in predicting the future power consumption of a city. We develop an encoder-decoder LSTM model, and this model performs significantly better with the geodemographic information. These findings are very useful for the energy companies. They can now use the geodemographic information of their consumers to design better energy management programs. They can also predict the electricity demand with greater accuracy. This will help them in achieving the demand-supply balance.

Stochastic Sampling on Bayesian Network-based Models for Document Ranking

Xing Tan

York University, Canada

Using approximate inference techniques, we investigate the applicability of Bayesian Networks to the problem of ranking a large set of documents. Topology of the network is a bipartite. Network parameters (conditional probability distributions) are determined through an adoption of the weighting scheme tf-idf. The rank of a document with respect to a given query is defined as the corresponding posterior probability, which is estimated through performing Rejection Sampling. Experimental results suggest that performance of the model is at least comparable to the baseline ones such as BM25. The framework of this model potentially offers new and novel ways of weighting documents. Integrating the model with other ranking algorithms, meanwhile, is expected to bring in performance improvement in document ranking.

Deep Neural Networks Are Effective At Learning High-Dimensional Hilbert-Valued Functions From Limited Data

Sebastian Moraga , Ben Adcock, Nick Dexter, Simone Brugiapaglia

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Recently, machine learning techniques based on Deep Neural Networks (DNNs) have begun to emerge as promising tools for function approximation in scientific computing problems, with some impressive results achieved on problems where the dimension of the underlying data or problem domain is large. In this work we consider Hilbert valued function approximation via Deep Neural Networks (DNN). This problem arises in many engineering problems, in particular those involving the solution of parametric PDEs. Such problems are challenging for three reasons. First, pointwise samples are expensive to acquire. Second, the domain of the function is usually high dimensional, and third, the range lies in a Hilbert space. Here we present a novel result on DNN training for holomorphic functions with so-called hidden anisotropy. This result introduces a DNN training procedure and a full theoretical analysis with explicit guarantees on the error and sample complexity. However, we also perform numerical experiments using different architectures and training. By fine-tuning the architecture and training scheme, we show that trained DNNs are able to outperform current best-in-class schemes on certain parametric PDE problems. This opens the door for further performance gains in the future.

Provably Accurate and Stable Deep Neural Networks for Imaging

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Deep learning has achieved key milestones in numerous image processing tasks, with recent developments and applications to linear inverse problems for imaging. For inverse problems, examples of imaging include modalities such as X-ray CT and MRI for medical imaging. Despite empirical results of deep learning achieving superior accuracy in this domain, a theoretical treatment ensuring the stability of deep neural networks is mostly absent in the current literature. In fact, such networks are vulnerable to adversarial attacks and are provably unstable under a reasonable linear inverse problem model, lacking a property known as kernel awareness.

In this talk, I will share our work in developing accurate and stable neural networks for imaging, which builds upon recent work by Adcock et al. (2021) and Antun et al. (2021). Our approach uses unravelling, a technique for constructing neural networks from convex optimization algorithms. I present a network construction through unravelling a restarted NESTA algorithm, utilizing a compressed sensing analysis to prove accuracy and stability of the network. The restarting enables exponential decay in network depth, yielding a shallower network. In turn this reduces computational costs, making the network feasible for practical purposes. Lastly, I discuss prospects of training stable deep neural networks for inverse problems in practice.

Mathematical Modelling for Transmission and Control of Infectious Disease 1

Organizer: **Pei Yuan, Jummy David**

Bayesian Inference and COVID-19

Adriana-Stefania Ciupeanu

Departments of Mathematics and Statistics, University of Manitoba, Canada

In this talk we will introduce Bayesian models and how we can use them for COVID-19.

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Numerically Modelling respiratory aerosol transport in indoor spaces, considering the implications of HVAC systems

Arma Khan, Marina Freire-Gormaly

Department of Mechanical Engineering, York University, Canada

Amid the COVID-19 pandemic, when considering the risk of indoor gatherings, concerns arise as to how the ventilation in indoor environments can prevent transmission of the COVID-19 infection through airborne routes. The ventilation techniques required to mitigate airborne transmission are unique to each space, and thorough research to determine the unique needs of various spaces is still lacking. The intended study will focus on developing a method to determine the risk factors associated with various heating, ventilation and

air-conditioning (HVAC) designs, complex room dimensions and dependence of index host location. The method consists of computational fluid dynamics (CFD) studies to determine possible transport phenomena in different conditions, and stochastically simulating the infection source location to determine the range of risk scenarios. After a verified method is developed to quantify risk factors, future work can incorporate various room dimensions, occupancies and HVAC designs to determine the risk factors associated with various spaces.

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Optimal public health responses to COVID-19 differ in high and low importation regions

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Public health responses to the COVID-19 pandemic have varied widely across the world. Some countries, or regions, have aimed for disease elimination, achieved through strict boarder control and periods of severe non pharmaceutical interventions (NPIs), while others have implemented suppression strategies, and imposed prolonged lockdowns to control community transmission. As NPIs have high economic costs, it is necessary to determine when elimination or suppression strategies are economically optimal. Although regions with higher importation rates may have higher infection prevalence, the relationship between the importation rate and the optimal implementation of NPIs has not been studied. Here we develop an epidemiological-economic model to determine when wither elimination or suppression strategies are optimal. We determine the intensity and timing of NPIs that minimizes the economic costs arising from the number of infections and NPI costs, for different importation rates, and in different economic regions. Economic regions are characterized by the ratio of daily NPI costs (expressed as a percent loss of the Gross Domestic Product (GDP) of a region) to the cost per infection. In our analysis, we consider this ratio to vary from 50 to 15,000, as this range of values is representative for Canadian provinces and territories. We found that if strict border control and fast detection of outbreaks can bring the importation rate close to zero, elimination strategies are a cost-effective strategy in minor as well as in small and large economies; otherwise suppression is the economically optimal choice. When suppression is best, optimal policies require restrictions to be gradually put in place as the number of infections increases, until a certain threshold is reached. The threshold should then be maintained by keeping the reproduction number R0 constantly below one. In large economies, optimal policies result in a higher number of active cases, and measures can be introduced more slowly. In these regions, reducing the importation rate has little impact on minimizing costs. In small economies, reducing importations allows for the implementation of less restrictive NPIs. This is because infection costs can lead to significant economic losses when regional GDP is low. In small economies, stricter measures need to be put in place to minimize community spread and optimize costs when the importation rate is high. Travel restrictions can therefore be considered a cost effective way to maintain lower alert levels in regions with smaller economies.

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Measuring the effect of behavior change during COVID-19 outbreak: Canada a case study

Yi Tan, Pei Yuan, Elena Aruffo, Huaiping Zhu

Centre for Diseases Modeling (CDM), York University, Canada
Department of Mathematics and Statistics, York University, Canada

The distinct ways of mitigating the COVID-19 pandemic have been unfolding in different countries and regions suggest that compliance with NPIs plays an important role. However, it is possible that the public does not always respect government recommendations, especially after one year of fighting with the disease. The state of public opinion and the degree of adhesion to an external given policy change with time is affected not only by the prevalence but also by people?s psychological activity. To evaluate how the severity of an epidemic is influenced by the distribution of adherence, the relative rates of disease dynamics, and the degree of irrational change behavior, we proposed a compartmental model incorporating behavioral change. The modelling results provide scientific evidence for the intricate interplay between human behaviors and disease prevalence, and highlight the importance of public education to adopt prevention measures and the need to avoid irrational changes.

Modelling Multiscale Systems in the Life Sciences

Organizer: **Harry J. Gaebler, Maryam Ghasemi**

An alternative delayed population growth difference equation model

Gail S. K. Wolkowicz, Sabrina Streipert

Department of Mathematics and Statistics, McMaster University, Canada

We propose an alternative delayed population growth difference equation model based on a modification of the Beverton?Holt recurrence, assuming a delay only in the growth contribution that takes into account that those individuals that die during the delay, do not contribute to growth. The model introduced differs from a delayed logistic difference equation, known as the delayed Pielou or delayed Beverton-Holt model, that was formulated as a discretization of the Hutchinson model. The analysis of our delayed difference equation model identifies a critical delay threshold. If the time delay exceeds this threshold, the model predicts that the population will go extinct for all non-negative initial conditions. If the delay is below this threshold, the population survives and its size converges to a positive globally asymptotically stable equilibrium that is decreasing in size as the delay increases. We show global asymptotic stability of the positive equilibrium using two different techniques. For one set of parameter values, a contraction mapping result is applied, while the proof for the remaining set of parameter values, relies on showing that the map is eventually componentwise monotone.

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Efficient sensitivity estimation for stiff stochastic discrete biochemical systems and applications

Monjur Morshed[a], Silvana Ilie[a], , Brian Ingalls[b]

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Numerous biochemical processes at the cellular level are inherently probabilistic, hence stochastic models must be employed to capture the random fluctuations observed in these systems. The Chemical Master Equation is a critical stochastic discrete model of biochemical systems. Models based on this formalism depend on physically motivated parameters, but frequently these parameters are not well constrained by

experiments. A fundamental tool in the study of biochemical systems is sensitivity analysis, which aims to measure the dependence of a system?s behaviour on model parameters. We propose a novel finite-difference technique for sensitivity estimation for discrete stochastic models of biochemical systems. The strategy is based on a variable time-stepping implicit tau-leaping scheme. This scheme is shown to have a reduced computational cost compared to previously published approaches for a similar accuracy, on models spanning multiple scales in time. In addition, this method can be applied for an efficient identifiability analysis of stiff stochastic biochemical systems.

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Beyond multiscale and multiphysics modeling in cellular biological media

George E. Kapellos

Department of Chemical Engineering, Massachusetts Institute of Technology, USA

Animal and plant tissues, microbial aggregates and biofilms, engineered tissues and cell-entrapping gels can be considered, under a unified perspective, as cellular biological media. In this regard, cellular biological media are defined as multiphase complex systems, which consist of biological cells along with their extracellular matrix, and exhibit a dynamically evolving and highly organized hierarchical structure. Theoretical modeling and computer simulation are indispensable tools for the analysis of transport and growth processes and, ultimately, the quantification of underpinning structure-function relationships in these biomaterials. Over the last two decades, a broad range of models has been developed based on principles from continuum mechanics and particle methods, many of which incorporate considerations across multiple scales of length, time and force. In this talk, the conceptual framework of existing models will be outlined and the potential of machine learning methods to capture the dynamic adaptation of cellular biological media will be explored.

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Emergent robustness of bacterial quorum sensing in fluid flow

Philip Pearce

Department of Systems Biology, Harvard University, USA

Bacteria use intercellular signaling, or quorum sensing (QS), to share in- formation and respond collectively to aspects of their surroundings. The autoinducers that carry this information are exposed to the external environment; consequently, they are affected by factors such as removal through fluid flow, a ubiquitous feature of bacterial habitats ranging from the gut and lungs to lakes and oceans. Here, we develop and apply a general theory that identifies the conditions required for QS activation in fluid flow by linking cell- and population-level genetic and physical processes. We predict that, when a subset of the population meets these conditions, cell-level positive feedback promotes a robust collective response by overcoming flow-induced autoinducer concentration gradients. By accounting for a dynamic flow in our theory, we predict that positive feedback in cells acts as a low-pass filter at the population level in oscillatory flow, allowing a population to respond only to changes in flow that occur over slow enough timescales. Our theory is readily extendable, and provides a framework for assessing the functional roles of diverse QS network architectures in realistic flow conditions.

Applications of Data Science in Financial Mathematics

Organizer: **Na Yu, You Liang**

Cubature Method for Volterra SDEs and Rough Volatility Model

Qi Feng

Department of Mathematics, University of Southern California, USA

The classical models for asset processes in math finance are SDEs driven by Brownian motion of the following type $X_t = x + \int_0^t b(s, X_s)ds + \int_0^t \sigma(s, X_s) \circ dB_s$. Then $u(t, X_t) = \mathbb{E}[g(X_T)|\mathcal{F}_t^X]$ is a deterministic function of X_t and $u(t, x)$ solves a parabolic PDE. The cubature formula is first constructed to numerically compute functionals like $\mathbb{E}^{\mathbb{P}}[g(X_T)]$, which can be seen as a discrete approximation of the infinite dimensional Wiener measure (denoted as $\mathbb{P}$). In this talk, we will consider that the asset process follows a rough volatility model. For example, in the rough Heston model, the process X_t is the solution of the Volterra type SDEs. In this case, X itself is non-Markovian, then $u(t, X_t)$ will depend on the whole path of $(X_s)_{0\le s\le t}$ and $u(t, X_{[0,t]})$ solves the so-called Path Dependent PDE (PPDE). We propose a new algorithm to numerically solve PPDE by using cubature type formulas for Volterra SDEs. The cubature formula for Volterra SDEs is solved by using machine learning method. In the end, I will show some numerical examples. The talk is based on joint work with Jianfeng Zhang.

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Novel Modelling Strategies for High-frequency Stock Trading Data

Xuekui Zhang

Department of Mathematics and Statistics, University of Victoria, Canada

High frequency trading stock data not only carry rich information and created new opportunities to better predict the mid-price, but also introduced new challenges for data analysis such as huge computational burden and high redundancy. Machine learning methods have been widely applied in stock mid-price movement prediction. However, how to smartly prepare input information for machine learning methods are not well investigated. In this work, we propose three novel strategies to utilize rich extra information in high-frequency data and address the new challenges. While these strategies can be used together with most machine learning methods, in this work, we illustrate them using Elastic Net. To show that our modelling strategies improve the prediction performance, results? interpretability, and robustness, we perform head-to-head experimental evaluations on real data of high frequency trading data of DOW 30 stocks.

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Systemic Risk in Repurchase Agreement Markets

Weijie Pang

Department of Mathematics and Statistics, McMaster University, Canada

The financial system is increasingly interconnected. Cyclical interdependencies among corporations may cause that a decision of one firm seriously affects other firms and even the whole financial network, which is a systemic risk. To describe the connections between banks, many researchers use the uncollateralized liabilities between two firms to construct financial network models to analyze the systemic risk. In practice, there are many collateralized liabilities between banks among the Repurchase Agreement (Repo) Market. Thus it is very important to include the Repo liabilities into a network model. In our research, we apply a Repo liability matrix and an uncollateralized liability matrix to describe the connections between banks. Based on this description, we construct different structures of banking balance sheets to quantify banks?

assets, liability and relationships to their counterparties. In a numerical study, we compare the effects of the collateralized and uncollateralized liabilities on the whole banking system under various financial shocks.

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A Novel Algorithmic Trading Strategy using Hidden Markov Model for Kalman Filtering Innovations

Ethan Johnson-Skinner

Department of Mathematics, Ryerson University, Canada

The development of algorithmic trading has been one of the most prominent trends in finance and its applications. In recent years there has been a growing interest in investigating the pairs trading and multiple trading based on robust Kalman filtering (KF) using data-driven innovation volatility forecasts (DDIVF). KF algorithms were successfully applied in pairs trading with two cointegrated assets using DDIVF as a method for forecasting non-normal innovation volatility. We propose a new pairwise trading strategy where a HMM is used in combination with DDIVF to further optimize trading signals in different market regimes. The results of the numerical experiments on two cointegrated stocks show that the proposed profitable trading strategy using DDIVF-HMM outperforms the recently studied robust trading strategy using DDIVF alone.

Mathematical Advances in Batteries 3

Organizer: **Iain Moyles, Matthew Hennessy**

DandeLiion: A ultra-fast solver for Doyle-Fuller-Newman models of lithium-ion battery discharge

Smita Sahu

University of Portsmouth, United Kingdom

DandeLiion (available at dandeliion.com) is a robust and extremely fast solver for the Doyle Fuller Newman (DFN) model, the standard electrochemical model for (dis)charge of a planar lithium-ion cell. DandeLiion conserves lithium, uses a second order spatial discretisation method (enabling accurate computations using relatively coarse discretisations) and is many times faster than its competitors. The code can be used 'in the cloud' and does not require installation before use. The difference in compute time between DandeLiion and its commercial counterparts is roughly a factor of 100 for the moderately- sized test case of the discharge of a single cell. Its linear scaling property means that the disparity in performance is even more pronounced for bigger systems, making it particularly suitable for applications involving multiple coupled cells. The model is characterised by a number of phenomenological parameters and functions, which may either be provided by the user or chosen from DandeLiion's library. This library contains data for the most commonly used electrolyte (LiPF6) and a number of common active material chemistries including graphite, lithium iron phosphate (LFP), nickel cobalt aluminium (NCA), and a variant of nickel cobalt manganese (NMC). We demonstrate DandeLiion's predictive power using a realistic drive cycle, and show that model solutions match experiment to within +/- 2%.

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Discerning Models of Phase Transformation in Porous Graphite Electrodes: Insights from Inverse Modelling Based on MRI Measurements

Jose Morales-Escalante

McMaster University, Canada

This work combines the techniques of inverse modelling with in-situ MRI measurements that were performed on a working graphite anode to investigate fundamental accuracy limitations of various models of Li transport within the insertion material. We augment the Newman model with two different descriptions of Lithium transport internal to the graphite, namely (non)linear diffusion and Cahn-Hilliard dynamics. These models are then calibrated via inverse modelling which identifies the transport properties (diffusivities in the diffusion model, or coefficients in the chemical potential in the Cahn- Hilliard model) leading to the best possible agreement between model predictions and measurement data. We find that a Fickian diffusion model is inadequate because it cannot accurately capture the sharp phase transitions of the graphite. We demonstrate that it is however possible to recover accuracy in a diffusion model by increasing its complexity and allowing the diffusivity to be a general function of concentration. When sufficient flexibility is allowed, the inverse modelling recovers a concentration-dependent diffusivity which is in qualitative agreement with the literature and exhibits significant ?dips? at values of the concentration known to correspond to a phase change. The Cahn-Hilliard model is also able to accurately fit the measurement data and it does so without the need to allow for state-dependence of its transport properties, indicating that it is overall a more economical choice for modelling intercalation into graphite. Our findings underscore the usefulness of performing model calibration simultaneously based on concentration and cell voltage measurements which can be efficiently done using methods of multi-objective optimization.

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Deep Neural Network Approximation of Li-ion Battery Models

Maricela McKay

Department of Applied Mathematics, University of British Columbia, Canada

Simplified models of Li-ion batteries like equivalent circuit models are inaccurate at high C-rates, while more comprehensive models like the Pseudo-two-dimensional model are too computationally expensive for use with most battery management systems. Additionally, accurate modeling requires that a parameter set for a given battery model be supplied. We present a framework for machine learning electrochemical models of Li-ion batteries. Our method uses a Feedforward Deep Neural Network (DNN) to approximate solutions of mathematical models of Li-ion batteries. This approach allows for underlying physical parameter dependencies to be learned, towards the goal of developing a general approximator for Li-ion batteries with adaptability to many battery chemistries. The RNN is trained with simulated driving cycles. Results show that good accuracy can be obtained from the ML approximation, avoiding the computational cost of the full electrochemical model once off-line training is complete. Additionally, we extend our approach with a recurrent neural network (RNN) to provide accurate state of charge estimates. Our approach shows promise for future applications to predicting battery failure and state of health estimates. This is joint work with Brian Wetton and Bhushan Gopaluni.

Novel and Unconventional Reaction–Diffusion Problems 3

Organizer: **Yana Nec, Justin Tzou**

The Tumor Invasion Paradox

Thomas Hillen, A. Shyntar, M. Rhodes

Department of Mathematical and Statistical Sciences, University of Alberta, Canada

The tumor invasion paradox relates to the artifact that a cancer that is exposed to increased cell death (for example through radiation), might spread and grow faster than before. The presence of cancer stem cell can convincingly explain this effect. In my talk I will use non-local and local reaction-diffusion type models to look at tumor growth and invasion speeds. We can show that in certain situations the invasion speed increases with increasing death rate ? an invasion paradox.

Resource-mediated competition between two plant species with different rates of water intake

Chunyi Gai

Department of Mathematics and Statistics, Dalhousie University, Canada

We propose an extension of the well-known Klausmeier model of vegetation to two plant species that consume water at different rates. Rather than competing directly, the plants compete through their intake of water, which is a shared resource between them. In semi-arid regions, the Klausmeier model produces vegetation spot patterns. We are interested in how the competition for water affects co-existence and stability of patches of different plant species. We consider two plant types: a ?thirsty? species and a ?frugal? species, that only differ by the amount of water they consume, while being identical in all other aspects. We find that there is a finite range of precipitation rate for which two species can co-exist. Outside of that range (when the rate is either sufficiently low or high), the frugal species outcompetes the thirsty species. As the precipitation rate is decreased, there is a sequence of stability thresholds such that thirsty plant patches are the first to die off, while the frugal spots remain resilient for longer. The pattern consisting of only frugal spots is the most resilient. The next-most-resilient pattern consists of all-thirsty patches, with the mixed pattern being less resilient than either of the homogeneous patterns. We also examine numerically what happens for very large precipitation rate. We find that for sufficiently high rate, the frugal plant takes over the entire range, outcompeting the thirsty plant.

Spike patterns as a window into non-injective transient diffusive processes

Yana Nec

Department of Mathematics, Thompson Rivers University, Canada

Complex natural systems at times manifest transitions between disparate diffusive regimes. Efforts to devise mea- surement techniques capable of identifying the cross-over moments have recently borne fruit, however interpretation of findings remains contentious when the bigger picture is considered. This study generalises the 1D Gierer-Meinhardt reaction ? diffusion model to a system that permits transitions between regular diffusive regimes with distinct dif- fusivities as well as sub-diffusion of a variable order. This is a sufficiently general, yet tractable description for the dynamics of a pattern qualitatively redolent of molecular clusters subject to transient anomalous diffusion mecha- nisms. The resulting system of equations substantiates the difficulties encountered when attempting to distinguish between various diffusive regimes in experimental settings: a non-monotonic dependence of the pattern?s evolution on parameters defining the diffusion mechanism is a common occurrence, as is a non-injective mapping between a given sequence of diffusion regimes and ensuing drift behaviour.

Dynamics of localized patchy vegetation patterns in the two-dimensional generalized Klausmeier model

Tony Wong, Michael Ward

Institute of Applied Mathematics, University of British Columbia, Canada

We discuss the dynamics and state-state behavior of localized spot patterns for the Klausmeier reaction-diffusion system. Through establishing a hybrid asymptotic-numerical theory, we analyze the existence, linear stability and slow dynamics of quasi-equilibrium and equilibrium spot solution in the singularly perturbed limit where the diffusivity of vegetation biomass is assumed to be much smaller than that of the water resource. Numerical simulations will be presented to verify our theory.

Utilizing AI and Machine Learning Techniques for Data Analytics 3

Organizer: **Wenying Feng, Jimmy Huang, Jianhong Wu**

Graph Neural Network Approach to Cross Lingual Entity Alignment

Sherry Zhu

York University, Canada

Cross-lingual entity alignment, which aims to match equivalent entities in KGs with different languages, has attracted considerable focus in recent years. Recently, many graph neural network (GNN) based methods are proposed for entity alignment and obtained promising results. However, existing GNN-based methods consider the two KGs independently and learn embeddings for different KGs separately, which ignore the useful pre-aligned links between two KGs. In this talk, we present some recent advances and progress have been made for the task of cross-lingual entity alignment, which is able to capture more cross-KG information through pre-aligned seed alignments and contextual information.

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Graph LSTM: Learning Graph Relationships in Spatiotemporal Data for Time Series Forecasting

Ryan Zhou

Queen's University, Canada

Spatiotemporal problems such as modeling vehicle flow are often approached by combining a spatial model, such as a graph neural network, with a temporal model such as LSTM. However, this approach presents two challenges: using a graph model requires defining the graph itself using domain knowledge, and the spatial and temporal models operate independently of one another, with only the spatial model making use of graphbased relationships. To address this, we propose an extension to the LSTM algorithm which adds a graph memory cell, allowing the model to learn from temporally distant events at other nodes without impacting its ability to model long-term relationships at a single node. We demonstrate using synthetic data that this model is capable of learning long-term patterns in other nodes. We then use the Graph Memory LSTM in a new model which learns node relationships by training edge weights directly. Experiments with this model on bike-share and traffic datasets show improved performance when compared to other models with similar numbers of parameters. We provide some insight into the sources of the improvements.

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Modeling Biases in Learning to Rank Systems

Jiashu (Jessie) Zhao

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In feeds recommendation, users are able to constantly browse items generated by never-ending items. The implicit feedback from users is an important resource for learning to rank, however, building ranking functions from such observed data is recognized to be biased. The presentation of the items will influence the user's judgements and therefore introduces biases. Most previous works in the unbiased learning to rank literature focus on position bias (i.e., an item ranked higher has more chances of being examined and interacted with). By analyzing user behaviors in product feeds recommendation, in this paper, we identify and introduce context bias, which refers to the probability that a user interacting with an item is biased by its surroundings, to unbiased learning to rank. We propose an Unbiased Learning to Rank with Combinational Propensity (ULTR-CP) framework to remove the inherent biases jointly caused by multiple factors. Under this framework, a context-aware position bias model is instantiated to estimate the unified bias considering both position and context biases. In addition to evaluating propensity score estimation approaches by the ranking metrics, we also discuss the evaluation of the propensities directly by checking their balancing properties.

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Adaptive sampling and domain learning strategies for multivariate function approximation on known and unknown domains

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We address the problem of approximating a smooth multivariate function defined on a general *domain of interest* from sample points. The domain may either be known in advance, or unknown and learned in the approximation process. This problem arises in various applications in scientific computing, in particular, surrogate model construction in UQ. It presents three main challenges: first, the *curse of dimensionality*; second, computing pointwise evaluation of f is expensive, and; third, the domain may be irregular, which may also be unknown *a priori*. First, for known domains, we study weighted least-squares approximation in an arbitrary space P from independent random samples taken according to a suitable measure. We present a new construction of a discrete sampling measure which leads to provably accurate and well-conditioned weighted least-squares approximations. Also, taking a sequence of nested spaces, we define a strategy, termed *Adaptive Sampling for General Domains (ASGD)*, that recycles the sample points in an adaptive way. Next, we consider domains that are unknown in advance. Here, our goal is to simultaneously approximate the function and learn the domain. We extend ASGD to this case, leading to a new method, termed *Adaptive Sampling for Unknown Domains (ASUD)*. We also extend ASGD to allow for other approximation schemes, such as compressed sensing and augmented least squares. Our numerical experiments show the benefit of ASUD over standard sampling techniques. Finally, we discuss how to combine the tools from ASGD and ASUD with deep learning for high-dimensional function approximation, leading to new, efficient sampling schemes for practical deep neural network approximation.

Mathematical Modelling for Transmission and Control of Infectious Disease 2

Organizer: **Pei Yuan, Jummy David**

Modelling the impact of viral traps on HIV-1 and SARS-CoV-2 infection

David W. Dick, Iain Moyles, Jane M Heffernan

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Successful management of human immunodeficiency virus (HIV) infection requires strict adherence to a daily drug regiment. The use of long-lasting red blood cell viral traps might offer an alternative that requires less frequent treatment offering a promising long-lasting augmentation to the existing highly active antiretroviral therapy (HAART).

Using impulsive differential equations, we model the in-host dynamics of HIV-1 infection and treatment with red blood cell viral traps. Our in-host model is informed from in-vitro experimentation of the neutralization of HIV-1 infection of TZMbl-cells. In this preliminary work, we seek to elucidate the requirements for successful use of red blood cell viral traps for both treatment of HIV-1 and prophylaxis against both HIV-1 and SARS-CoV-2 infection.

The Effects of Adherence to Antiretroviral Therapy for HIV-1 Infection

Lauren Clara Browning McKenzie, Stacey Smith?

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The emergence of drug resistance is a serious threat to the long-term virologic success and durability of HIV-1 therapy. Adherence has been shown to be a major determinant of drug resistance; however, each pharmacologic class of antiretroviral drugs has a unique adherence–resistance relationship. We develop an immunological model of the HIV-1 infected human immune system that integrates the unique mechanisms of action of reverse transcriptase and protease inhibiting drugs. A system of impulsive differential equations is used to examine the drug kinetics within $CD4^+$ T cells. Stability analysis was preformed to determine the long-term dynamics of the model. Using the endpoints of an impulsive periodic orbit in the drug levels, the maximal length of a drug holiday while avoiding drug resistance is theoretically determined; the minimum number of doses that must be subsequently taken to return to pre-interruption drug levels is also established. Heterogeneity in inter-individual differences on drug-holiday length is explored using sensitivity analysis based on Latin Hypercube Sampling and Partial Rank Correlation Coefficient analysis. Extremely short drug holidays are acceptable, as long as they are followed by a period of strict adherence. Numerical simulations demonstrate that if the drug holiday exceeds these recommendations, the cost in virologic rebound is unacceptably high. These theoretical predictions are in line with clinical results and may also help form the basis of future clinical trials.

Age group Model construction for COVID-19 Transmission with Vaccination

Donglin Han, Michael Li, Weston Roda, Marie Varughese, Qun Cheng

Department of Mathematical and Statistical Sciences, University of Alberta, Canada

In this presentation, we'll talk about how to construct a mathematical model for Alberta COVID-19 with vaccination in an age-specific way. We introduce parameters not related to vaccination such as health-seeking behaviour parameter and birth and death rates, we also talk about parameters related to vaccination such as vaccination rates and efficacy of vaccines.

Modelling the COVID-19 epidemic and interventions during the first wave in Alberta

Qun Cheng, Michael Li, Weston Roda, Marie Varughese, Qun Cheng

Department of Mathematical and Statistical Sciences, University of Alberta, Canada

Ending the global SARS-CoV-2 pandemic requires multiple interventions, including social distancing, testing and contact tracing. In collaboration with Alberta Health, we have applied a mathematical model to predict the scale and dynamics of the epidemic and estimate the effectiveness of public health interventions, and inform public health responses in Alberta. The model consists of three compartments: susceptible (S), infected (I), reported cases (R), for three age groups (0-18 year, 19-64 years, and 64 years and older). Contact mixing matrix among the age groups and time-dependent case-infection ratio are considered in the model. Estimation of model parameters are obtained by fitting the model to past COVID-19 data (May-March 2020) from Alberta Health using Bayesian inference and Markov Chain Monte Carlo (MCMC) sampling. (The presentation is based on collaborative research between Dr. Michael Li's research group and Alberta Health)

Contributed Talks

Session 1

The effect of movement behavior on population density in fragmented landscapes

Nazanin Zaker Frithjof Lutscher Laurence Ketchemen Tchouaga

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Landscape fragmentation arises from human activities and natural causes and may create abrupt transitions (interfaces) in landscape quality. How landscape fragmentation affects ecosystems diversity and stability depends, among other things, on how individuals move through the landscape. In this work, we focus on the movement behavior at an interface between habitat patches of different quality. Specifically, we study how this individual-level behavior affects the steady state of a density of a diffusing and logistically growing population in two adjacent patches.

We consider a model for population dynamics in a habitat consisting of two homogeneous one-dimensional patches in a coupled ecological reaction diffusion equation. The movement between patches is incorporated into the interface conditions. We establish the existence, uniqueness, and global asymptotic stability of the steady state. Then we explore how the qualitative properties of the steady state depend on movement behavior.

We apply our analysis to a previous result where it was shown that a randomly diffusing population in a continuously varying habitat can exceed the carrying capacity at steady state. We clarify the role of nonrandom movement in this context. In particular, we determine conditions on movement rates and patch preference, so that the steady-state density exceeds the carrying capacity.

Competition dynamics of seasonal breeders

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Many species are discrete (annual) breeders who, between reproductive events, consume resources and may die. Their resource often reproduces continuously or has short, overlapping generations. An accurate model for such life cycles needs to represent both, the discrete and the continuous processes in the community.

I will present a basic model for a single consumer and its resource in a two-season environment. I will give some basic properties of the model and explain how it differs from the purely continuous and the purely discrete analogues that have been studied for many decades. Then I will introduce competing species and consider coexistence mechanisms for many discrete-breeder consumers on a single limiting resource. The model shows that a large number of consumers can coexist at attractors of various complexity.

A framework for studying transients in marine metapopulations

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Transient dynamics can often differ drastically from the asymptotic dynamics of systems. In this talk we provide a unifying framework for analyzing transient dynamics in marine metapopulations, from the choice of norms to the addition of stage structure. We use the ℓ_1 norm, because of its biological interpretation, to extend the transient metrics of reactivity and attenuation to marine metapopulations, and use examples to compare these metrics under the more commonly used ℓ_2 norm. We then connect the reactivity and attenuation of marine metapopulations to the source-sink distribution of habitat patches and demonstrate how to meaningfully measure reactivity when metapopulations are stage-structured.

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Moving Habitat Models: A Numerical Approach

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We present a system of reaction-diffusion equations to model population dynamics within climate-driven moving habitats. We generalize current models by including habitat dependent dispersal rates, habitat preference and by allowing the habitat to move at various speeds. The assumptions on individual movement behaviour result in a jump in density across habitat types. We build and numerically validate a finite difference scheme to study the transient dynamics, and, when they exist, steady-state solutions. Our numerical scheme uses a conformal moving mesh and a modification of the finite difference scheme to capture the jumps in density. We apply our scheme to two ecologically relevant climate-shifting scenarios: constant nonmatching speeds and accelerating speeds. In the former, we find that a strong preference for the suitable habitat helps the population persist at faster shifting speeds, yet sustains a smaller total population at slower shifting speeds. In the latter, we find that a high preference for the suitable habitat at lower acceleration rates increases the time to extinction but decreases the time to extinction at higher acceleration rates.

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Population density in fragmented landscapes under monostable and bistable dynamics

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A model for a single species population which propagates in a heterogeneous landscape in a one dimensional space is presented. The landscape is composed of two kind of patches with different diffusivities. The dynamics of the population is studied through a reaction diffusion model on which the net growth function can be a monostable or bistable function. In addition, we consider that at the interface between patch types,

individuals may show preference for more favorable regions. We study the different nonlinear steady state models. We prove existence of monotone solution in each model and classify their qualitative shape. An analysis is done to study the effect of the diffusivity coefficient. A stability analysis is also done for each model.

Accurate Approximation of Models of the Spread of Infectious Diseases

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Since the identification of the COVID-19 epidemic in 2019, there has been an intensive global research effort devoted to improving the accuracy and reliability of mathematical models of the spread of infectious diseases. International experts in computational biology and computational medicine have developed such models and most of the models that have been proposed involve systems of ordinary differential equations (ODEs) and some data data fitting.

In this presentation, we will consider models based on an underlying classical SIR epidemic model, and we will show how dramatic improvements in accuracy and reliability of their approximate solutions can be obtained by employing carefully chosen robust numerical methods to integrate the ODEs that arise. In particular the ODE method must be able to automatically detect and handle delay terms and discontinuities that are often associated with these models.

We show, using an example of modelling a COVID-19 outbreak, that our approach is able to efficiently determine an accurate simulation of a real epidemic over different accuracy requests (without making strong assumptions on the problem or data). In this example we use a reliable, order six, continuous Runge Kutta method (SDC_CRK6) developed by our research group to solve the systems of ODEs.

Cigarette smoking on college campuses: an epidemical modelling approach

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A compartmental model depicting the spread and cessation of the smoking habit on college campuses is formulated and analysed. A sensitivity analysis indicates that Rc is most sensitive to the contact rate between habitual-smokers and occasional-smokers and cigarette quitting rate. Numerical simulations of the proposed optimal control strategies reveal that the most effective approach to reduce the prevalence of cigarette smoking and possibly achieve a smoking-free campus should combine both control measures.

Session 2

On Mathematics of Financial Markets and Contracts

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In the talk some aspects of financial market modeling and of option pricing will be considered. We provide a new look at the classical Bachelier model making stock prices non-negative. The most well-known transformation of this type is exponential, and it leads to the Geometrical Brownian Motion or the Black-Scholes model. We develop here another method of getting such modifications which is based on Stochastic Differential Equations with absorption and reflection. In the framework of these modifications of the Bachelier model we discuss problems of perfect and imperfect hedging of European options. Formulas of quantile and CVaR-hedging will be derived. Moreover, it will be shown how these results are applied in the areas of regulatory capital and life insurance.

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Conservative Hamiltonian Monte Carlo

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In Bayesian statistics, MCMC methods enable effective sampling of complex posterior distributions, which results from a combination of previously known information (the prior) and data (the likelihood). Traditionally, MCMC methods sample the posterior distribution by utilizing a random walk with a rejection and acceptance criteria at each iteration. This process will converge to the target posterior distribution provided the acceptance and rejection criteria are chosen correctly relative to the prescribed random walk. However, the acceptance rate inevitably diminishes as the dimension of the posterior increases. This has led to recent developments in computational techniques, such as Langevin Monte Carlo and Hamiltonian Monte Carlo (HMC), to improve the performance in convergence and acceptance rate. While HMC relies on volume-preserving numerical integrators to effectively sample from the target posterior distribution, the acceptance rate of the algorithm depends heavily on the (approximate) energy-preserving properties of the chosen numerical integrator. In this talk, we introduce the Conservative Hamiltonian Monte Carlo (CHMC) method, where instead of employing a volume-preserving integrator, we utilize an energy-preserving integration technique known as the Discrete Multiplier Method. We show that CHMC converges to the correct posterior distribution under appropriate conditions and provide numerical examples showcasing improvements on acceptance rates when compared to HMC.

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On the dynamics of coupled Mathieu equations

Jiuda Wu, Behrooz Yousefzadeh, Payam Azadian

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Parametrically excited systems are widely used in engineering and physics, in applications ranging from large power systems to microelectromechanical amplifiers. Parametrically excited waveguides have recently received significant attention in photonics and material design due to their asymmetric wave propagation characteristics: the transmission properties depend on the direction of the propagating waves. This

lack of symmetry, also known as breakdown of reciprocity, can enable steady regimes of asymmetric wave propagation in modulated waveguides, with application in communication devices and vibration isolation. Modulated waveguides are typically modeled as an infinite series of Mathieu equations, which are then analyzed asymptotically in the limit of weak parametric excitation. Recent experimental realizations of modulated waveguides in mechanical systems, however, operate beyond these limits. To bridge this gap between the operating regimes of theory and experiments, we study the nonreciprocal dynamics of coupled Mathieu equations at moderate excitation levels. We discuss the role of the phase difference between adjacent oscillators, as well as the influence of nonlinearity, on the nonreciprocal bias of the system. While our focus is mainly on the dynamics of two coupled oscillators, we discuss the influence of the number of units, thereby making connections with the theory of modulated waveguides.

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Where Models Fail: Stationary Probability Distributions of Stochastic Gradient Descent and the Success and Failure of the Diffusion Approximation

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In this research, Stochastic Gradient Descent (SGD), an optimization method originally popular due to its computational efficiency, is analyzed using Markov chain methods. We compute both numerically, and in some cases analytically, the stationary probability distributions (invariant measures) for the SGD Markov operator over all step sizes or learning rates.The stationary probability distributions provide insight into how the long-time behavior of SGD samples the objective function minimum, and could ultimately be useful in characterizing generalization errors in supervised learning problems.

A key focus of this research is to provide a systematic study in one dimension comparing the exact SGD stationary distributions to the Fokker-Planck diffusion approximation equations Ñ which are commonly used in the literature to characterize the SGD probability distribution in the limit of small step sizes/learning rates. While various error estimates for the diffusion approximation have recently been established, they are often in a weak sense and not in a strong maximum norm. Our study shows that the diffusion approximation converges with a slow rate in the maximum norm to the true stationary distribution. In addition to large quantitative errors, the exact SGD probability distribution exhibits fundamentally different behavior to the diffusion approximation: for example, they can have compact or singular supports; and there can be multiple invariant measures for non-convex objective functions (when the diffusion approximation only has one).

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The role of temperate bacteriophages in the maintenance and distribution of Antibiotic Resistance Genes (ARGs).

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Bacteriophages or simply phages are the viruses that infect bacteria. Temperate phages can insert their genome into the host bacterial genome; the inserted phage is termed a prophage. Prophages are subject to mutational degradation over time, but may also be maintained by selection if they confer benefits to

their bacterial hosts. These prophages can excise from the bacterial genome randomly or in response to environmental cues or DNA damaging agents, killing the bacterial host and restarting the process of transmission and infection. The highly mobile nature of phages makes them frequent agents of horizontal gene transfer (HGT).

Phage genomes often carry antibiotic resistance genes (ARGs). These ARGs can be retained in the prophage stage if they confer a selective benefit to the host, and their mobility makes them a potential ÒreservoirÓ of ARGs. The ability of phages to transfer between bacteria poses a significant risk in the global transmission of antimicrobial resistance.

We applied a combination of bioinformatics, analytical modeling, and computational simulation approaches to understand the diverse gene content of prophages. We analyzed genes in 1384 prophages. The data indicate that while some genes (involved in the replication, packaging, and release of phage particles) are significantly lost, others (tail fiber, transposase, and integrase genes) are significantly enriched. The results of our ODE model and gene-level simulations are in agreement with prophage repertoire data. The gene-level simulations also explain the spread and maintenance of ARGs in the temperate phages.

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Functional Kernel Density Estimation: Point and Fourier Approaches to Time Series Anomaly Detection

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We present an unsupervised method to detect anomalous time series among a collection of time series. To do so, we extend traditional Kernel Density Estimation for estimating probability distributions in Euclidean space to Hilbert spaces. The estimated probability densities we derive can be obtained formally through treating each series as a point in a Hilbert space, placing a kernel at those points, and summing the kernels (a Òpoint approachÓ), or through using Kernel Density Estimation to approximate the distributions of Fourier mode coefficients to infer a probability density (a ÒFourier approachÓ). We refer to these approaches as Functional Kernel Density Estimation for Anomaly Detection as they both yield functionals that can score a time series for how anomalous it is. Both methods naturally handle missing data and apply to a variety of settings, performing well when compared with an outlyingness score derived from a boxplot method for functional data, with a Principal Component Analysis approach for functional data, and with the Functional Isolation Forest method. We illustrate the use of the proposed methods with aviation safety report data from the International Air Transport Association (IATA).

Session 3

Limit processes and bifurcation theory of quasi-diffusive perturbations

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The bifurcation theory of ordinary differential equations, and its application to deterministic population models, are by now well established. In this article, we begin to develop a complementary theory for

diffusion-like perturbations of dynamical systems, with the goal of understanding the space and time scales of fluctuations near bifurcation points of the underlying deterministic system. We then discuss the application of this theory to stochastic population models in a well-mixed setting.

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The electric double layer at the interface between a polyelectrolyte gel and a salt bath

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Polyelectrolyte gels consist of a network of electrically charged, deformable polymer chains that are swollen with fluid. These gels are typically surrounded by a salt bath, which allows for solvent and ion exchange until an equilibrium is established. The migration of ions towards the gel-bath interface leads to the formation of a diffuse, electrically charged layer called an electric double layer (EDL). Starting from a new phase-field model that accounts for the nonlinear elasticity of the gel, we use matched asymptotic expansions in combination with numerical methods to resolve the EDL at the gel-bath interface. By applying our framework to cylindrical geometries, we show that the conventional scenario where a thin EDL forms at the surface of an electrically neutral gel only arises if solvent gradients are heavily penalised by a large interfacial energy. Otherwise, phase separation occurs in the EDL and propagates into the bulk, leading to the emergence of heterogeneous gels composed of repeating, electrically charged domains with varying degrees of swelling. We argue that special care must be taken when interpreting experimental data using electroneutral models of polyelectrolyte gels, which is common in the literature.

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How stable are sliding viscoplastic films?

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When a fluid film spreads with little traction over a surface, the main resistance to flow stems from the extensional stresses of the material, in contrast to flow above a no-slip surface where shear stresses dominate. Experiments with radially spreading sliding viscous films have suggested these flows are stable towards non-axisymmetric disturbances. However, the analysis of the stability of radially expanding two-dimensional flow of a shear-thinning power-law fluid suggests the presence of an extensional flow instability. In this talk we extend this analysis to three-dimensional spreading films with a viscoplastic (yield-stress) rheology. Considering the thin-film limit, we construct axisymmetric base states and then test their stability towards non-axisymmetric perturbations by numerically solving the initial-value problem. We complement the numerical analysis with analytical solutions for early and late times. The analysis confirms the existence of instability and suggests it is particularly strong at late times, where the spreading of the base state becomes self-similar, if the fluid has a yield stress or is sufficiently shear-thinning.

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Well-balanced schemes for modelling multi-component transport in two-dimensional shallow water flow

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We propose well-balanced numerical schemes for solving coupled systems modelling the transport of multiple passive scalars in shallow water flows over variable topography. A well-balanced discretization of the source term due to variable topography is introduced. New techniques are developed to satisfy the positivity required for some physical parameters of the system such as the computed water depth and the scalar concentrations. We prove the well-balanced property of the proposed numerical schemes and the positivity of the scalar concentration for each component of the mixture constituents. Numerical experiments are performed to test the robustness and accuracy of the proposed method. The results of our numerical tests confirm stability, well-balanced properties for the water surface elevation and the concentrations, as well as the positivity preserving property for both the computed water depth and scalar concentrations of the mixture constituents. The developed schemes can be used to predict the solutions of coupled systems modelling water flows and the transport of multicomponent passive scalars.

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A positivity-preserving numerical scheme satisfying the discrete maximum-minimum principle for surface water flow and solute transport

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In this study, we develop a well-balanced positivity-preserving unstructured numerical method for modelling the coupled system of shallow water flow and solute transport with source terms due to variable bottom topography, bottom friction effects and diffusion. New well-balanced positivity preserving discretization techniques are developed for the water surface elevation and the scalar concentration. In the absence of source terms of the passive pollutant, the constant concentration states are preserved in space and time over complex topography for any hydrodynamic field of the flow. Novel discretization technique for the diffusion term is proposed to ensure the positivity of the scalar concentration. Piecewise linear reconstructions techniques are proposed for the water surface elevation and concentration to ensure the discrete maximum-minimum principle for the solute concentration. Our techniques are validated using numerical examples, where we test the well-balanced and positivity properties of the proposed numerical method and its robustness in predicting the solutions of the coupled model of shallow water flow and solute transport.

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Interfacial instabilities in a Hele-Shaw cell

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The Hele-Shaw cell consists of a thin gap between two parallel plates, along which fluid is forced to flow to provide a constrained geometry suitable for experimental and theoretical study. When one fluid is pumped through the cell to displace a second fluid, the interface between them can, in some cases, develop in an unstable fashion. The Newtonian Saffman-Taylor problem is one such example that has been well studied, predicting an instability driven by the viscosity difference between the two fluids. When the less viscous fluid displaces the more viscous one, the interface is unstable; but if the more viscous fluid displaces the less viscous one, the interface remains stable. The goal of the current study is to explore and analyse two other types of instabilities. The first one is the viscoplastic version of the Saffman-Taylor instability, replacing the displaced Newtonian fluid with a yield stress fluid. The second one is a fracturing instability that occurs when water is displaced by a yield stress fluid. In this configuration, the theory predicts no Saffman-Taylor instability and therefore a stable interface, because the viscoplastic fluid has a higher effective viscosity than water. However, instead of growing asymmetrically, the interface fractures and leads the flow into flower-like shapes.

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Theory and Experiment of Preferential Loop Fractions of Polymers Adsorbed to Silica Nanoparticles

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A discrete combinatorial model was constructed to find if there is a preference for a higher loop-fraction on a system of adsorbed polymer chains to a surface, where a loop is a segment of the polymer chain that only touches the surface at the two endpoints of the segment. The model parameters were based on experiment, where the polymer chains were that of polyacrylic acid polyelectrolyte (PAA) with a chain length of 6200 monomers. These chains were adsorbed to a silica nanoparticle and fully covered the surface. The polymer and loop configurations were represented as self avoiding walks and self avoiding polygons respectively. A combinatorial approach was used to locate the preference of fraction of looping of the attached polymers.This was achieved through finding the amount of looping per polymer that makes the greatest contribution to the partition function. This research will provide insights on controlling the biophysical properties of materials and surfaces relevant to tailoring biocompatibility and biomimetics useful in the medical industry.

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Nonlinear SAR imaging via convexification inversion method

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In contrast with the conventional algorithms of synthetic aperture radar (SAR) imaging, which works with the linearized scattering mathematical model, the fully nonlinear inverse scattering problem for a hyperbolic equation is considered. An inversion scheme, based on the convexification method is proposed to approximate the dielectric constants of hidden objects in the 2D and 3D domains. The global convergence of the method is established. Numerical tests were conducted on experimentally collected data.

Session 4

Unsteady Ideal Gas Flow Through Porous Media

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Landfill gas flow as a fluid flow field has attracted the attention of fluid dynamics researchers only recently. This man-made system is unique in its combination of disparate flow regimes, counter-intuitive responses to control parameters and inherent uncertainty in all other parameters. This talk focuses on the temporal variation of the suction strength imposed to extract the gas as well as surface boundary conditions. Darcy's law subject to the weak compressibility of the fluid results in a non-linear partial differential equation for the pressure field. Slow variation admits asymptotic solutions for generic time dependence of the boundary forcing function, both as Dirichlet and Neumann conditions. Flow control strategies are discussed based thereon. A sealed outer domain boundary is identified as the configuration best amenable to full control of the pressure profile via the induced well suction. Fast variation leads to a novel application of the classical compact support similarity solution in a domain with discontinuous parameters. It is shown that the asymptotics obtained for the slow regime encompass most realistic scenarios, from truly slow to fast, whereas the mathematically fast regime solution is only required for situations mimicking Dirac delta type evolution. The results are also applicable to natural gas collection and sparging wells.

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Modeling Turbulence in Landfill Gas Flow: Ingress into a Horizontal Well

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Landfill gas collection is a salient component of waste management, energy recovery and environmental protection. The objective of the study is to improve the design and efficiency of operation of horizontal collection wells from the aspect of flow turbulence. Flow within the porous landfill mass is coupled to free pipe flow. Past studies performed this coupling without addressing the turbulence at the ingress to the well apertures. However, investigation near the apertures showed local fluctuations in pressure indicative of the importance of proper turbulence modeling. COMSOL Multi-physics simulation software is used to couple Darcy flow in the porous media with Navier-Stokes equations within the well using two turbulence closure models. The results are compared to semi-analytical solutions implemented in Octave/Matlab. Significant discrepancy in head losses within the well was observed between the two approaches. The cumulative ingress impact is shown to decrease the suction strength required for adequate gas extraction. Differences in the Reynolds number variation showed the limitation of the quasi-1D geometry employed in the semi-analytical solutions. The velocity profiles at the ingress revealed the importance of mesh refining and careful ingress flow modeling. The comparison of friction factor within the well proved the impact on the pressure was solely due to turbulence effects at the ingress. Pressure profiles within the landfill mass showed that the majority of head losses occurs over a very small ingress vicinity. The study conclusively proves the importance of including turbulence at the ingress for a realistic representation of flow in the horizontal well.

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A space-time spectral method for the Stokes problem

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In this work, we consider the Stokes equations in steady and unsteady states, along with Dirichlet boundary conditions and an initial condition in the latter case. We impose the $\mathbb{P}_N - \mathbb{P}_{N-2}$ spectral Galerkin scheme in space by using a recombined Legendre polynomial basis resulting in exponential convergence in space. For the unsteady state, we implement spectral collocation in time, thus giving exponential convergence in both space and time. The global spectral operator for both schemes is a saddle point matrix. We prove the 2-norm estimates for every block of the two operator matrices, and proceed to show that the condition number for the global spectral operator for the steady-state scheme is $\mathcal{O}(N^4)$, where N is the number of spectral modes in each direction. We also have results on the condition number of the unsteady-state scheme. Numerical results of this scheme applied to the unsteady Navier-Stokes problem will also be shown.

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Space-time localized radial basis function method for modelling water flow in porous media

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The process of infiltration of water through soils can be described using the Richards model. In this study, we develop space-time mesh-free numerical techniques for efficiently solving the Richards equation. The proposed techniques combine two advantages which are related to the use of a local multiquadric radial basis function method avoiding mesh generation and the use of a space-time technique which allows us to design an efficient numerical scheme in terms of computational cost. The local mesh-free techniques are more flexible in dealing with complex geometries and irregular boundaries and present many advantages in terms of system conditioning where we obtain a sparse matrix for the resulting system. This has the advantage of using reduced memory and computational time and the space-time technique has the benefit of solving the resulting algebraic system only once compared to standard numerical methods. To demonstrate the performance of the proposed techniques, a series of numerical examples are performed in two-, three- and four-dimensional space-time regular and irregular domains. Our numerical simulations confirm the accuracy, efficiency in terms of computational cost, and capability of the proposed numerical method in predicting the dynamics of unsaturated flow through soils.

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Local factorization of multidimensional discrete differential operators

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We present a novel approach to factoring discrete approximations to the Laplacian in multidimensional space using the “grid algebra” approach. The goal is to accelerate the computational speed of implicit solution methods for numerical partial differential equations. The “implicit” part typically requires a computationally intensive step of calculating the solution to a high dimensional linear system that involves both the current and future states of the system, and it is this step that we are able to accelerate. The results here consider the shifted discrete Laplacian and its discrete approximations, expressed as an affine combination of sufficiently many independent finite difference operators, which is then factored as product of an upper triangular matrix and its adjoint, using only nearest neighbour coefficients. This Affine Local Grid Factorization (ALG-F) results in a linear system that is rapidly solved via two instances of back substitution. The result is an implicit scheme that is O(N) rather than the typical O(N^2) of traditional implicit finite difference schemes.

We demonstrate the method with numerical implementations of the ALG-Factorization to solve the acoustic wave equation in two and three dimensions for both directionally symmetric and non-symmetric grid spacing. Extensions to N-dimensions and stability results will be established.

This work is a report of MSc thesis research completed by RJ Vestrum in 2021.

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Quasi-Geostrophic Magnetohydrodynamics

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The quasi-geostrophic magnetohydrodynamic (QG-MHD) equations can describe the evolution of a relatively thin layer of plasma, in the limit of strong rotation (Zeitlin, 2013). While this limit is characterized by small Rossby number, these equations can be reduced to those of standard two-dimensional magnetohydrodynamics in the opposing limit of infinite external deformation radius, where the starÕs rotation (for example) has no effect on the motion. Turbulent flows are often characterized by the way energy is distributed between the length scales of the motion (namely, their energy spectrum). A direct (inverse) cascade is one where energy moves to smaller (larger) scales .

It is established in the literature that in the absence of rotational forces, decaying QG-MHD turbulence has a direct energy cascade (Orszag and Tang, 1979; Pouquet,1978). The energy spectrum is anticipated to follow a ?3/2 spectral slope in the inertial range, following a modification of KomolgorovÕs argument (Iroshnikov, 1963; Kraichnan, 1965). In this work, we compare the energy spectra of both decaying turbulence and an unstable jet in both the presence and absence of rotational forces. In particular, we computationally confirm Kraichnan and IroshnikovÕs expected slope (as did Biskamp and Welter (1989)) and further consider the effects of a small but non-zero Rossby number. We additionally compute the spectral energy fluxes to confirm the direction of the energy cascade and compare the different regimes.

Session 5

Implicit and semi-implicit second-order time stepping methods for the Richards equation

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We consider numerical methods for efficiently solving the Richards equation where different weak formulations and computational techniques are analyzed. The spatial discretizations are based on standard or mixed finite element methods. Different implicit and semi-implicit temporal discretization techniques of second-order accuracy are studied. To obtain a linear system for the semi-implicit schemes, we propose second-order techniques using extrapolation formulas and/or semi-implicit Taylor approximations for the temporal discretization of nonlinear terms. A numerical convergence study and a series of numerical tests are performed to analyze efficiency and robustness of the different schemes. The developed scheme, based on the proposed temporal extrapolation techniques and the mixed formulation involving the saturation and pressure head and using the standard linear Lagrange element, performs better than other schemes based on the saturation and the flux and using the Raviart-Thomas element. The proposed semi-implicit scheme is a good alternative when implicit schemes meet convergence issues.

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Stochastic Runge-Kutta pseudo-symplectic methods

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Symplectic schemes show better accuracy in numerical simulations over a long time interval, but unless we consider a special type of stochastic Hamiltonian systems, they are implicit methods, so the computing time is large. Pseudo-symplectic methods are explicit methods that preserves the symplectic structure up to a certain order of accuracy, so they offer a compromise between the long-term accuracy and the computing time. Pseudo-symplectic schemes based on generating functions require many derivatives of high order of the Hamiltonian functions. To deal with this issue, here we construct explicit Runge-Kutta pseudo-symplectic schemes. Our approach is based on a rooted tree analysis and stochastic B-series for order condition.

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Accurate defect estimation for continuous numerical solutions of ordinary differential equations

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Current high-quality software packages for the numerical solution of differential equations must return continuous numerical solution approximations for which some form of error control is implemented. It is important that the error control be applied to the continuous approximate solution. In this talk, we will discuss a new software package for the numerical solution of ordinary differential equations that features direct control of the defect (or residual) of the continuous numerical solution based on the use of high-order optimal Runge-Kutta methods and associated high-order interpolants. The package employs asymptotically correct defect control. Issues associated with the representation of the basis polynomials upon which the interpolants are based, that arise for computations were high accuracy is required, will be examined. We show that the use of Barycentric-Lagrange representations for the basis polynomials can lead to substantial improvements in the quality of the defect estimates.

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A high-order moment limiter for the discontinuous Galerkin method on triangular meshes

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In the presence of discontinuities, numerical solutions of hyperbolic conservation laws obtained using the discontinuous Galerkin method often develop oscillations. These oscillations can lead to numerical instabilities and eventual degradation of solution quality. Slope limiting is one of the techniques used to suppress such spurious oscillations. We present an arbitrarily high-order moment limiter for the discontinuous Galerkin method on unstructured triangular meshes in this work. The limiter works by hierarchically reconstructing directional derivatives along specific directions and limiting solution coefficients by comparing them to the computed derivatives. Limiting along these directions is performed using a one-dimensional minmod limiter. We use a compact stencil consisting of only eight mesh elements to reconstruct the directional derivatives and the stencil can be computed in the pre-processing stage. We present numerical examples to show that limited solutions are robust in the presence of discontinuities and retain the theoretical rate of convergence for smooth solutions.

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Numerical Computation of the Tracy-Widom Distribution

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Recently, random matrix theory has become one of the most exciting fields in probability theory, and has been applied to problems in high dimensional data analysis, wireless communications, finance, etc. The Tracy-Widom distribution, describing the normalized largest eigenvalue of a random Hermitian matrix, is one of the most important probability distributions in random matrix theory.

In the first half of the talk, we will give an overview of existing numerical methods for evaluating the Tracy-Widom distribution, including methods based on solving an ordinary differential equation, and approximating a Fredholm determinant. In the second half of the talk, we will give an introduction to a new method, which also approximates a Fredholm determinant, and is based on exploiting a pair of commuting differential and integral operators. Our new method evaluates the distribution to full absolute precision everywhere rapidly, including in both tails. Moreover, it evaluates the right tail of the distribution to full relative precision.

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Superlinear convergence of BFGS method by using Kantorovich type assumptions

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Consider the solution of a nonlinear system of equations. Almost all convergence theory for quasi-Newton methods assume the existence of a root and bounds on the nonlinear function and its derivative in some neighborhood of the root. However, these conditions cannot be checked in practice. Kantorovich's version of convergence theory for NewtonÕs method only makes assumptions about a neighborhood of the initial point, and the existence of a solution and the rate of convergence are consequences of the theory. The motivation of this talk is to derive a Kantorovich-type convergence theory for Broyden, BFGS, and scaled memoryless BFGS method where all assumptions can be verified, and the existence of a root and its superlinear rate of convergence are consequences of the theory. The theory is simple in the sense that it contains a few constants as possible. The other part of this talk extends this theory for unconstrained minimization problems. We consider Perry's nonlinear conjugate gradient method and prove superlinear local convergence of this method by using Kantorovich-type hypotheses. Only the basic version of these methods without line search is considered.

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Various Numerical Methods for the Microscopic Cardiac Electrophysiology Model

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To study propagation at the level of cardiac myocytes, the microscopic model ex- plicitely represents individual cells. The cardiac tissue is then viewed as two separate domains: the intra-cellular and extra-cellular domains, respectively $\frac{1}{2}$ i and $\frac{1}{2}$ e separated by cellular membranes ?. The microscopic model consists in a set of Poisson equations, one for each sub-domain $\frac{1}{2}$ i and $\frac{1}{2}$ e , coupled on interfaces ? with nonlinear transmission conditions involving a system of ODEs. Few numerical methods are available in the literature for the microscopic model. We discretize this problem in space using finite element methods, that may be conformal or non-conformal on the interface ?. We then propose and compare various time-stepping methods for solving the microscopic model, among which the Godunov splitting method, first and second order implicit and semi-implicit methods. Godunov splitting leads to the solution of two sub-problems, namely the nonlinear ODE models representing the ionic activity on ? and coupled linear space propagation problems on $\frac{1}{2}$ i and $\frac{1}{2}$ e . The other methods addresses fully coupled linear or nonlinear discrete problems. Error estimates are obtained, proving the order of the methods in time. Numerical results are presented to compare the stability, accuracy and efficiency of the methods.

Posters

Circadian regulation of the immune system and sexually dimorphic effects of shiftwork

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Shift work has a negative impact on health and can lead to chronic diseases and illnesses. Under regular work schedules, rest is a night time activity and work a daytime activity. Shift work relies on irregular work schedules which disrupt the natural sleep-wake cycle. This can in turn disrupt our biological clock, called the circadian clock, a network of molecular interactions generating biochemical oscillations with a near 24-hour period. Clock genes regulate cytokines before and during infection and immune agents can also impact the clock function. We provide a mathematical model of the circadian clock in the rat lung coupled to an acute inflammation model to study how the disruptive effect of shift work manifests itself in males and females during inflammation. Our results show that the extent of sequelae experienced by male and female rats depends on the time of infection. The goal of this study is to provide a mechanistic insight of the dynamics involved in the interplay between these two systems.

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Modeling Turbulence in Landfill Gas Flow: Ingress into a Horizontal Well

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Landfill gas collection is a salient component of waste management, energy recovery and environmental protection. The objective of the study is to improve the design and efficiency of operation of horizontal collection wells from the aspect of flow turbulence. Flow within the porous landfill mass is coupled to free pipe flow. Past studies performed this coupling without addressing the turbulence at the ingress to the well apertures. However, investigation near the apertures showed local fluctuations in pressure indicative of the importance of proper turbulence modeling. COMSOL Multi-physics simulation software is used to couple Darcy flow in the porous media with Navier-Stokes equations within the well using two turbulence closure models. The results are compared to semi-analytical solutions implemented in Octave/Matlab. Significant discrepancy in head losses within the well was observed between the two approaches. The cumulative ingress impact is shown to decrease the suction strength required for adequate gas extraction. Differences in the Reynolds number variation showed the limitation of the quasi-1D geometry employed in the semi-analytical solutions. The velocity profiles at the ingress revealed the importance of mesh refining and careful ingress flow modeling. The comparison of friction factor within the well proved the impact on the pressure was solely

due to turbulence effects at the ingress. Pressure profiles within the landfill mass showed that the majority of head losses occurs over a very small ingress vicinity. The study conclusively proves the importance of including turbulence at the ingress for a realistic representation of flow in the horizontal well.

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Optimal bath particle density selection for Reactive Multiparticle Collision dynamics

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Particle-based numerical methods are able to accurately and efficiently simulate the evolution of biochemical reaction-diffusion systems. One particular algorithm, Reactive Multiparticle Collision (RMPC) dynamics, performs well on systems with approximately-homogeneous species distributions within the simulation domain. However, it can be challenging to maintain constant diffusion throughout the simulation domain with RMPC in instances where particle concentrations are strongly inhomogeneous, and even more so when species diffuse at different rates. The use of inert 'bath' particles to ensure more uniform diffusion rates has shown great promise in mitigating this difficulty, but a method to ascertain the required density of these particles is needed.

We present initial work towards a comprehensive method to select suitable bath particle densities, based on two different primary approaches. The first attempts to automatically infer an optimal homogeneous bath density for each species conditioned on data describing the desired overall behaviour, using progressively-narrowing parameter sweeps. This optimal point is unique, and we show that selecting a bath density above or below it results in decreased simulation accuracy. The second explores the utility of an inhomogeneous bath density specification for severely-inhomogeneous systems, with emphasis on the accuracy-performance trade-off.

In summary, we show the existence of an optimal bath particle density for some strongly-inhomogeneous systems, and propose an automatic method to locate it. When this approach is not successful, we show that using an inhomogeneous bath density gives good results, but can be computationally expensive.

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Narrow Capture Problems: Trap Arrangements Minimizing Average Mean-First Passage Time in the Unit Sphere and Unit Ellipse

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The determination of statistical characteristics for particles undergoing Brownian motion in constrained domains has applications in various areas of research. This work presents attempts to systematically compute globally optimal configurations of traps inside a both two- and three-dimensional domains that minimize the average of the mean first passage time (MFPT) for the narrow capture problem, the average time it takes a particle to be captured by any trap. For a given domain, the mean first passage time satisfies a linear Poisson problem with Dirichlet-Neumann boundary conditions. While no closed-form general solution of such problems is known, approximate asymptotic MFPT expressions for small traps in a unit sphere have been found. These solutions explicitly depend on trap parameters, including locations, through a pairwise

potential function. Global optimization was performed to find optimal trap positions in the unit sphere, and ellipses of varying eccentricity, for identical traps. The interaction energy values and geometrical features of the putative optimal trap arrangements are presented.

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Is This an Emergency or a Usual Visit to the DoctorÕs office? Modeling Electronic Health Records (EHR) with Irregular Intervals of visits

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EHR provide valuable insights on the progression and identification of various diseases, however, patients tend to visit the doctor's office in irregular time intervals. Numerous time series models such as Auto-Regressive Integrated Moving Average (ARIMA) models require constant timespans and therefore one of the approaches has been to interpolate the values and turn uneven timespans into uniform ones. This approach introduces biases and loss of information such as not distinguishing an important event that the irregular time series elicits. For instance, a patient with an emergency that undergoes surgery has to visit the doctor more frequently due to that event versus another patient who has a more stable condition and visits the doctor on a more regular basis: these two patients have different information in their time series which the uniform model does not draw out. Our aim is to introduce and compare models such as Recurrent Neural Networks and Hidden Markov Models that can consider the irregular intervals of visits in EHR and to predict the outcome of specific lab exams using these models.

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Parallel computing of a viscoplastic fluid in an annular model

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In this research, we studied the narrow eccentric annuli model for a Herschel-Bulkley fluid developing an implementation in parallel using the graphic processor unit (GPU) technology and the development of an optimal algorithm for the annuli model. The result of this research takes the contribution of different fields, particularly two very specialized areas: Non-Newtonian fluid dynamics and high-performance computing. From the Non-Newtonian fluid dynamics point of view, the motivation of the study of the eccentric annuli considering a laminar flow using a Hele-Shaw approach which has its physical motivation from the industrial process of primary cementing used to complete oil wells prior to production. Given the complexity of the model, the computational cost of a solution with the real-life parameter is very expensive in terms of memory capacity and speed of the processor. Many authors have contributed to redesign the algorithm and reduce the computational time. This work reduces the time of execution significantly using a GPU and also optimizing the algorithm itself. We identified what part of the code spent more resource and time with a detailed analysis of code using specialized software tools for that. As in many cases, a very complex problem is reduced to a simple calculation several times. In this case, intensive and recursive usage of a root finder slowed down the code severely, hence a massive change in the way this was calculated was performed. We showed that optimum usage of hardware and software could improve the general performance of a program with several industrial applications.

Sparse Random Wavelet Signal Representation and Decomposition

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A novel method for sparsely representing and decomposing 1D signals will be presented. This method involves solving the Basis Pursuit Denoising (BPDN) problem of representing a signal as a sparse sum of randomly generated Gabor wavelets with different time shifts, frequencies, and phases before clustering the wavelets into different modes based on their time shift and frequency. Applications to Blind Audio Source Separation (BASS) in music will be demonstrated.

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Effects of promoter methylation on the period of a minimal circadian clock model

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The circadian (about a day) clock strikes a balance between robust intrinsic rhythmicity and plasticity to environmental cues. At a cellular level, interconnected transcription-translation feedback loops produce reliable limit cycle oscillations in core clock proteins. Although there has been extensive mathematical modelling, important questions remain about the effects of environmental signals on the molecular circadian clock. For instance, recent experiments suggest that DNA modification at gene promoters plays a role in stably altering the circadian period. In this poster, we present and analyze an extension of a minimal model of the circadian clock. By including an additional degree of freedom in the classical mixed feedback loop model of Francois and Hakim, we analyze how an additional promoter state alters the dynamics of the clock. We obtain conditions for equilibrium uniqueness and an asymptotic approximation to the clockÕs period, which allow us to bound the influence of the new promoter state in our model. We then use another set of approximations to connect our model to a modified version of the Goodwin oscillator, previously studied in this context by Kim and Forger. Analysis of this reduced model reveals that although epigenetic factors can alter the period, they may also result in a loss in rhythmicity. Our analysis adds a quantitative perspective to an active area of biological research and offers several avenues for future work.

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Epithelial transport during pregnancy in the rat nephron

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Normal pregnancy is characterized by a significant plasma volume expansion and sodium retention in rats and many mammals including humans. This expansion is critical for supplying the demand of a growing uterus and fetus through gestation. Kidneys are essential in fluid balance in the body so large changes are made to support the changes in plasma volume and solute retention required during gestation. Disordered

pregnancy, including preeclampsia, as well as fetal growth restriction is marked by failure to expand the plasma volume so understanding renal function during pregnancy is needed for effective treatments of these gestational diseases. In this work we develop an epithelial transport mathematical model of a female rat nephron for a mid-pregnant and late-pregnant rat. The model accounts for the changes that happen in the abundance of apical and basolateral transporters, single nephron glomerular filtration rate, and tubular dimensions during mid- and late- pregnancy.

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