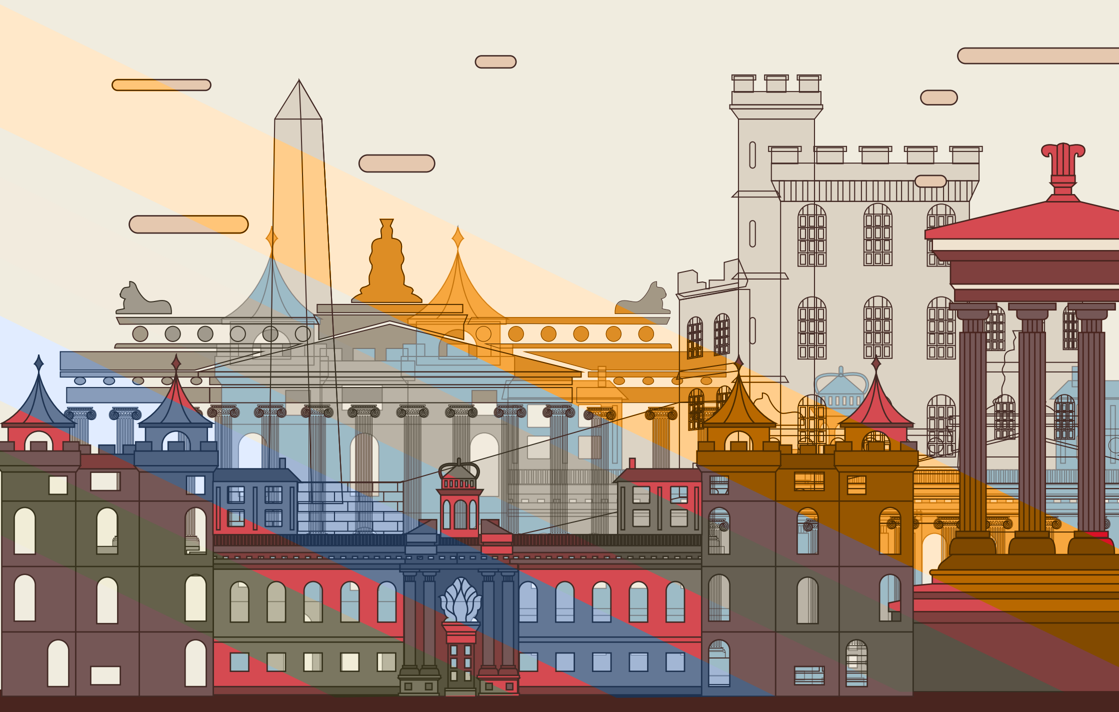
10TH SIAM UKIE National Student Chapter Conference

June 23 - 24, 2022

Hosted by
The Edinburgh SIAM – IMA Student Chapter



Book of Abstracts

10TH

SIAM UKIE National Student Chapter Conference

June 23 - 24, 2022

EDINBURGH - SCOTLAND

10th SIAM UKIE National Student Chapter Conference

June 23 – 24, 2022

Edinburgh, Scotland

Organizing Committee

Jonna Roden (Chair) • Matthew Holden • Savvas Melidonis • Andrés Miniguano-Trujillo

Maxwell Institute for Mathematical Sciences, Edinburgh, Scotland

Funding Institutions

Society for Industrial and Applied Mathematics *(SIAM)* • The Institute of Mathematics and its Applications *(IMA)* • International Centre for Mathematical Sciences *(ICMS)* • Maxwell Institute Graduate School in Analysis and its Applications *(MIGSAA)* • The University of Edinburgh • Heriott–Watt University

Edited by

Andrés Miniguano-Trujillo

Edinburgh City Skyline in Cover by

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Presentation

The Edinburgh SIAM-IMA Student Chapter is excited to welcome you to the 10th SIAM UKIE National Student Chapter Conference (NSCC) taking place at the University of Edinburgh from June 23-24, 2022. This event marks the first time that a Scottish university will host the yearly meeting. The NSCC is a two-day conference that features four plenary speakers, 24 talks by Ph.D. students, and student poster presentations on the evening of the first day. It is held completely in person at The University of Edinburgh, 50 George Square, rooms G.04 and G.05.

Our aim is to strengthen the connection of Edinburgh's PhD student community with those of the UKIE student chapters. We would like to provide opportunities to early career researchers to present their work and to network with our invited plenary speakers and with other early career researchers from across the UK and Ireland.

Further details on the conference are available in this booklet and on the conference website. If you have any questions, find one of us at the conference venue, or email us at `siam-ima@maths.ed.ac.uk`.

We are looking forward to great presentations by the plenary and contributed speakers and hope you will have an amazing time in Edinburgh!

All the Best,

Andrés, Jonna, Matthew, Savvas
The Edinburgh SIAM-IMA Student Chapter Committee

About us

The Edinburgh SIAM-IMA Student Chapter consists of PhD students from the University of Edinburgh and Heriot Watt University and jointly represents the Society for Industrial and Applied Mathematics (SIAM) and the Institute for Mathematics and its Applications (IMA). Our aim is to bring students from the two universities together, as well as to provide them with opportunities to connect with other SIAM Chapters, and to academic and industry communities.

Program

Time UTC+1	Thursday	
10:00-10:30	**Coffee & Registration**	
10:30-11:30	**Plenary Talk:** Professor Gabriela Gomes – G.04	
11:30-12:30	**Student Talks**	
	fORum Session [TPS1] – G.04	Parallel Session 2 [TPS2] – G.05
12:30-14:00	**Lunch Break**	
14:00-15:00	**Student Talks**	
	Parallel Session 3 [TPS3] – G.04	Parallel Session 4 [TPS4] – G.05
15:00-15:45	**Coffee Break**	
15:45-16:45	**Plenary Talk:** Professor Martin Schmidt – G.04	
17:00-18:30	**Poster Session & Wine Reception**	
19:00	**Conference Dinner**	

Time UTC+1	Friday	
09:30-10:30	**Plenary Talk:** Dr Małgorzata Zimoń – G.04	
10:30-11:00	**Coffee Break**	
11:00-12:00	**Student Talks**	
	MIGSAA Session [FPS1] – G.04	Parallel Session 1 [FPS2] – G.05
12:00-13:30	**Lunch Break**	
13:30-14:30	**Student Talks**	
	Parallel Session 3 [FPS3] – G.04	Parallel Session 4 [FPS4] – G.05
14:30-14:45	**Coffee Break**	
14:45-15:15	**Closing Ceremony & Prize Announcements**	
15:15-16:00	**Walk around Edinburgh**	

Plenaries

Frailty Variation in Population Dynamics: Adventures and Disadventures of an Elusive Concept

Gabriela Gomes • University of Strathclyde, UK • gabriela.gomes@strath.ac.uk

Thursday, 23/06/2022, 10:30-11:30 (UTC+1)

Selection acting on unmeasured individual variation is a common source of bias in the analysis of populations. It has been shown to affect measured rates of mortality, the survival of endangered species, the scope of neutral theories of biodiversity and molecular evolution, measured risks of diseases whether non-communicable or infectious, the efficacy of interventions such as vaccines or symbionts, and it may be an underappreciated cause for the reproducibility crisis that the life and social sciences currently travers.

Forms of variation that respond to selection and impact population dynamics, termed frailty variation in demography, remain elusive in many disciplines. I will present some examples, including how this appears to have affected the course of the coronavirus disease (COVID-19) pandemic.

Multilevel Optimization: Basics, an Application to the European Gas Market, and an Open Research Problem

Martin Schmidt • Trier University, Germany • martin.schmidt@uni-trier.de

Thursday, 23/06/2022, 15:45-16:45 (UTC+1)

In this talk, we will give an introduction to the field of multilevel optimization. To this end, we first focus on bilevel optimization problems and study their main properties. By doing so, we will see why this class of problems are very important for practice but we will also see why they are very challenging - both from a theoretical and from a practical point of view. Afterward, we discuss a recent application of multilevel optimization to model the European gas market as well as present and discuss some exemplary results for real-world data. Finally, we will illustrate how practical models need to be extended to cover uncertain aspects as well. This leads to a rather novel class of bilevel optimization problems for which we pose the open research question on whether they can be solved on a computer anyway.

The Path Towards Experimentation by Simulation... is Paved with Surrogate Models

Małgorzata Zimoń • IBM Research, UK • Malgorzata.Zimon@uk.ibm.co

Friday, 24/06/2022, 09:30-10:30 (UTC+1)

Digital twin can be defined as a composable virtual representation of a system that can span its life cycle, is continuously updated from design and operational data, and can use simulation, machine learning, and reasoning to augment decision-making and / or control the system. Recent advances in computational workflows, physics-based solvers, big data processing and management tools bring the promise of digital twins and their impact on society closer to reality. One important enabling technology is surrogate modelling. The basic idea in the surrogate model approach is to invest resources in developing fast mathematical approximations to the long running computer codes or expensive physical experiments. Given these approximations, many questions can be posed and answered, many trade-offs explored, and insights gained. In this presentation, I will discuss different types of surrogate models and how they can be utilised advantageously in digital twin framework. I will focus on two areas: uncertainty quantification and system prediction for industrial applications.

TBA

Andrew Duncan • Imperial College London & Improbable, UK • a.duncan@imperial.ac.uk

Friday, 23/06/2022, 14:30-15:30 (UTC+1)

Savvas please.

Contributed Student Talks

Contents

TPS1 — Parallel Session 1

fORum Session

fORum (Seminar for PhD Students in Optimisation and OR) is a hybrid seminar for PhD students in Optimisation and Operational Research from the School of Mathematics at the University of Edinburgh. The purpose of this activity is to create a community of practice where PhD students in this discipline can get valuable input for their research, stay up to date with advances in the field and stay informed about different applications outside of their topic. fORum seminars usually consist of research talks by our PhD students, and industry talks by guest speakers with experience working in OR teams in different industries. As part of seminars, joint events with research groups from other universities are organised with the goal of establishing and strengthening relationships between PhD students in Optimisation and OR across universities and countries.

HiGHS - An Edinburgh Optimization Success Story

Ivet Galabova • The University of Edinburgh, Scotland • ivet.galabova@ed.ac.uk

Thursday, 23/06/2022, 11:30-11:50 (UTC+1)

HiGHS offers high performance open-source linear optimization software that is becoming increasingly popular with users, interface developers and more general software systems, and the overall performance of HiGHS on LP (simplex and barrier) and MIP problems now exceeds that of any other open-source software. This talk will discuss recent developments in HiGHS, and introduce some application areas where its performance and open-source philosophy are particularly highly valued.

How Can we Speed up Solving a Large-scale Distributed Energy Portfolio Management Problem?

Monserrat Guedes Ayala • The University of Edinburgh, Scotland • s1553571@ed.ac.uk

Thursday, 23/06/2022, 11:50-12:10 (UTC+1)

The energy industry is quickly shifting towards decarbonised ways of producing electricity and the available technologies that facilitate such progress are in constant development and evolution. This has caused an expansion of energy portfolios since they now include assets such as solar, wind or hydroelectric generation, as well as different types of energy storage systems. Each of these assets has their own characteristics and limitations, but they must all be modelled and operated jointly, together with market interactions, to minimise total costs of running energy portfolios. Modelling these interactions simultaneously increases the complexity and dimensionality of the problem of optimally managing these distributed energy resources, making solution approaches computationally expensive. This is problematic since energy markets move fast and agents are required to constantly make decisions such as how much to buy from the market, how much to sell, or how much to store in available batteries. This presentation explores different problem-specific ways in which we can speed up the computational time of solving this class of problems, with a special focus on improving open-source solvers through decomposition techniques.

Interior Point Methods for Optimization Problems Arising in Imaging and Optimal Transport

Filippo Zanetti • The University of Edinburgh, Scotland • f.zanetti@sms.ed.ac.uk

Thursday, 23/06/2022, 12:10-12:30 (UTC+1)

In this talk we discuss how interior point methods (IPMs) can be applied to large scale optimization problems and how they perform with respect to first order methods; in particular, two applications are considered. The first one is an IPM for tomographic imaging with a novel regularization that tries to separate the two materials in the object; the quadratic term is large and dense and can only be accessed through matrix-vector products; we present theoretical results in terms of choice of the regularization parameters and eigenvalue bounds for the preconditioned matrix, as well as experimental data. The second application is a sparse IPM for discrete optimal transport problems, where the constraint matrix is of huge dimension but highly sparse and structured; we present a theoretical result about the sparsity structure of the optimal solution that allows us to mix iterative and direct solvers efficiently, as well as experimental results.

TPS2 — Parallel Session 2

Modelling the Just-right Hypothesis of Tumorigenesis

Xell Brunet Guasch • Maxwell Institute for Mathematical Sciences, Scotland •
xell.brunetguasch@ed.ac.uk

Thursday, 23/06/2022, 11:30-11:50 (UTC+1)

It is well established that tumour progression benefits from genetic instability by generating cellular diversity, including genetic alterations that allow overcoming barriers such as escaping checkpoints or increasing proliferation (Hanahan & Weinberg, 2000). The “just-right” model of tumorigenesis states that, whilst a certain level of genomic instability and/or mutation accumulation is necessary for tumour growth, too high levels might be harmful and potentially lead to tumour extinction. A clear understanding of this phenomenon is lacking, and has the potential to guide therapeutic strategies exploiting the 'too much' end of genomic instability. We propose the use of branching processes (Athreya & Ney, 1972; Haccou, Jagers, & Vatutin, 2005) to model the underlying evolutionary dynamics, coupling theoretical work with input from on-going experiments and genomics. In my presentation, I will be discussing preliminary work on two models that study the mutation limit.

The first model, based on (McFarland, Mirny, & Korolev, 2014), is a birth-death process in which, after division, a cell might acquire a driver mutation, which provide a strong selective advantage driving tumour growth, or a mildly deleterious mutation, which provide a weak selection disadvantage. The growth of a subpopulation depends on the number of mutations of each type. Preliminary results show that, if enough mildly deleterious accumulate, their multiplicative fitness reduction effects have a large enough impact to cause tumour extinction.

The second model, based on (Solé & Deisboeck, 2004), considers a more general cell failure, where high mutation rate is lethal as an error catastrophe. We model this as a birth-death process of three populations: healthy cells, mutator cells and genomically unstable cells, where the fitness of the latter is a decreasing function of mutation rate. Preliminary results show an intermediate range of mutation rates in which the probability of a tumour progressing is maximal.

Both our models and experimental work by colleagues (Soriano et al., 2021) indicate a strong dependency between tumour fate and mutation rate. In practice, mutation rate does not only vary considerably between tumours, but also varies as a tumour evolves. Our next goal is to gain understanding of how variation in mutation rate over time might shapes tumour dynamics, and its interplay with the just-right hypothesis.

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Source Optimisation for Brachytherapy Radiation Problems

Jenny Power • University of Bath • jip30@bath.ac.uk

Thursday, 23/06/2022, 11:50-12:10 (UTC+1)

Brachytherapy is a cancer treatment where radioactive sources are placed directly onto the tumour to be treated. These sources are in the form of seeds of radioisotopes that decay, releasing radiation to eradicate the tumour. However, when the tumour is located close to critical organs, the radiation emitted may damage these organs, causing further health complications. A challenge lies in positioning the sources such that the tumour is exposed to the required amount of radiation to eradicate it, but the critical organ is not exposed to excessive toxicity. This is the challenge this research tackles. The problem is formulated as a PDE constrained optimisation problem. The PDE constraint is a radiation transport equation that outputs the radiation dose distribution in the domain when given the source locations. A prescribed dose is assigned to the tumour region. The objective function is designed such that when minimised, the radiation dose in the tumour matches the prescribed dose and that the dose outside of the tumour is minimised. This is implemented as a numerical model using continuous Galerkin finite elements.

A Trade-off Between Two Tolerance Strategies of the Host Leads to Evolutionary Branching

Prerna Singh • University of Sheffield • psingh2@sheffield.ac.uk

Thursday, 23/06/2022, 12:10-12:30 (UTC+1)

There are crucial distinctions between tolerance to the effects of infection-induced deaths (mortality tolerance) and tolerance to the parasite-induced reduction in the reproduction of infected hosts (sterility tolerance). Theoretical studies have discussed the negative correlation between tolerance and resistance mechanisms, but such a correlation within different modes of tolerance is rarely looked upon. Here we consider a host population subjected to a pathogen that adversely affects both aspects of the host's fitness; fecundity and mortality. We assume that the host responds by evolving tolerance to both forms of parasitic impact and obeys a sterility-mortality tolerance trade-off. So, increasing mortality tolerance comes at the cost of lowered sterility tolerance and vice versa.

We have extended a classic host-parasite SIR model and used adaptive dynamics framework to model the evolution of two forms of tolerance as host defense strategies. Existing theory claims that a direct trade-off within two defense strategies do not allow evolutionary branching unless there is an additional cost to some host life-history trait. However, we discovered that a trade-off between two tolerance strategies drives the host population to branch into extreme dimorphic strains, i.e., branching occurs. As such, the strain in which infected hosts are sterile but have low mortality can coexist with the strain in which infected hosts are fully fertile and have a high mortality rate.

In this talk, I will discuss the conditions in which such a trade-off leads to the occurrence of dimorphic strains and how evolution drives the patterns of disease prevalence in the host population.

TPS3 — Parallel Session 3

A Bayes Linear Emulation Approach for the Qualitative and Quantitative Inputs

Muhammad Mahmudul Hasan • Durham University • mahmudul.sta@du.ac.bd

Thursday, 23/06/2022, 14:00-14:20 (UTC+1)

One of the rising issues of complex computer experiments is finding a suitable way of modelling the qualitative and quantitative inputs together. Some approaches are already developed for addressing the qualitative and quantitative inputs problem by using Gaussian processes. Although some of the existing methods used the constant mean for their analysis procedure; some others only consider the single factor input and all of them exclude the nugget effect entirely. An alternative way of handling complex computer experiments is using Bayes linear emulation, but this has only been used for quantitative inputs so far. This work proposes a novel approach for solving the rising issue considering the Bayes linear emulation approach with the nugget effect rather than the Gaussian approach. We explore a variety of correlation structures to represent the mixed quantitative and qualitative natures of the input variables, and finally combine this with the Bayes linear approach to construct an emulator for qualitative and quantitative inputs. We applied our proposed method over a complex Environmental Policy Integrated Climate (EPIC) computer simulator with both quantitative inputs (fertiliser levels) and qualitative inputs (soil type, steepness, and weather), and which can simulates crop yield for 80 different crops over a 100 year period. We have also performed the robustness analysis and used different existing diagnostic tools to check the validity of our proposed mixed inputs Bayes linear emulation approach.

Unifying Information Propagation Models and Their Influence Maximisation

Yu Tian • University of Oxford • yu.tian@maths.ox.ac.uk

Thursday, 23/06/2022, 14:20-14:40 (UTC+1)

Information propagation is a central theme in social, behavioural, and economic sciences, with important theoretical and practical implications, such as the influence maximisation problem for viral marketing. There are two widely adopted models in this context: the independent cascade model where nodes adopt their behaviour from each neighbour independently, and the linear threshold model where collective effort from the whole neighbourhood is needed to influence a node. However, both models suffer from certain drawbacks, including a binary state space, where nodes are either active or not, and the absence of feedback, as nodes can not be influenced after having been activated previously. To address these issues, we consider a model with continuous variables that has the additional advantage of unifying the mechanisms underlying these two classic models. For the associated influence maximisation problem, the objective function is no longer submodular, a feature that most approximation algorithms are based on but is arguably strict in practice. Hence, we develop a framework, where we formulate the influence maximisation as a mixed integer nonlinear programming and adopt derivative-free methods as general solutions. Furthermore, we show that the problem can be exactly solved in the special case of linear dynamics, and propose a customised direct search method accordingly, with local convergence. We demonstrate the rich behaviour of the newly proposed information propagation model and the close-to-optimal performance of the customised direct search method numerically on both synthetic and real networks.

Reinforcement Learning for Optimal Execution

Huining Yang • University of Oxford • huining.yang@maths.ox.ac.uk

Thursday, 23/06/2022, 14:40-15:00 (UTC+1)

Optimal execution of large positions over a given trading period is a fundamental decision-making problem for financial services. In this talk we explore reinforcement learning methods, in particular policy gradient methods, for finding the optimal policy in the optimal liquidation problem. We show results for the case where we assume a linear quadratic regulator (LQR) model for the underlying dynamics and where we apply the method to the data directly. The empirical evidence suggests that the policy gradient method can learn the global optimal solution for a larger class of stochastic systems containing the LQR framework, and that it is more robust with respect to model mis-specification when compared to a model-based approach.

TPS4 — Parallel Session 4

Properties of the Eigenfunctions of the SFS Operator with $\alpha = 0$

Farhana Akond Pramy • The Open University • farhana.pramy@open.ac.uk

Thursday, 23/06/2022, 14:00-14:20 (UTC+1)

I have been working on the Stretch-Fold-Shear (SFS) operator S_α which is a functional linear operator acting on complex-valued functions of a real variable x on some domain containing $[-1, 1]$ in $\mathbb{R}$. It arises from a stylized model in kinematic dynamo theory. When the shear parameter α is zero, the spectrum of S_α can be determined exactly. Using generating function methods, properties of the eigenfunctions of S_α can be obtained in the case $\alpha = 0$. These eigenfunctions are related to the Bernoulli polynomials and have similar properties. In the talk I shall show how the generating function gives the eigenfunctions, show how they are related to the classical Bernoulli polynomials and give some of the properties of the eigenfunctions.

A Minimal Phase-Coupling Model for Intermittency in Turbulent Systems

Enda Carroll • University College Dublin • enda.carroll@ucdconnect.ie

Thursday, 23/06/2022, 14:20-14:40 (UTC+1)

Turbulent systems exhibit a remarkable multi-scale complexity, in which coherent, intense, and rare events in the velocity gradients induce scale-dependent statistics with strong departures from Gaussianity – a phenomenon known as intermittency. Correspondingly, in Fourier space, phase correlations can give rise to complex scale-dependent properties, as the one developed in the presence of coherent shocks. A quantitative relation between real-space structure, statistics, and phase synchronization is currently missing. Here, we address this problem in the framework of a minimal phase-coupling model which enables a detailed investigation by means of dynamical systems theory and multi-scale high-resolution simulations. The model is formulated in terms of Fourier phases whose dynamical coupling resembles the one in Navier-Stokes turbulence. Specifically, it is Burgers turbulence with the important distinction that the amplitudes are kept at fixed values such that only the Fourier phases evolve. By changing the spectrum slope α we can tune the coupling strength of the phases and study how the intermittency of the underlying velocity field changes. We find that both very steep and very shallow spectra exhibit close-to-Gaussian statistics, while strong departures from Gaussianity are observed for intermediate slopes comparable to the ones in hydrodynamic and Burgers turbulence. We show that the non-Gaussian regime of the model coincides with a collapse of the dynamical system to a lower-dimensional attractor and the emergence of phase synchronization, thereby establishing a dynamical-systems perspective on turbulent intermittency.

Hybrid Modelling of Secondary Droplet Dynamics

Oscar Holroyd • University of Warwick • o.holroyd@warwick.ac.uk

Thursday, 23/06/2022, 14:40-15:00 (UTC+1)

High-speed liquid drop impacts can, under the right conditions, produce significant volumes of ejecta able to travel long distances. The evolution of these secondary droplets is of particular interest in the context of pesticide spraying, oil-spill dispersion, and icing prevention.

Numerically modelling these dynamics poses a significant challenge. The physics governing the impact's dramatic topological changes takes place at the microscale. However, in the seconds after impact the ejected droplets can spread over distances on the order of metres. Applying state-of-the-art direct numerical simulations to this second phase is not computationally feasible, and so we switch to a more appropriate framework: a kinetic model.

Here we propose a novel smoothing region to bridge the gap between DNS and kinetic models, allowing us to dramatically reduce the computational cost of modelling the system, while retaining the benefits of the two paradigms.

FPS1 — Parallel Session 1
MIGSAA Session

The Maxwell Institute Graduate School in Analysis and its Applications (MIGSAA) is a Centre for Doctoral Training in analysis and the applications of analysis to a wide range of areas. MIGSAA has funded 5 cohorts of 12 students between 2014 and 2018, with PhDs awarded jointly by both the University of Edinburgh and Heriot-Watt University. Since the last cohort is graduating in 2022, a MIGSAA farewell event is held in three sessions, showcasing work in pure and applied analysis, as well as probability. The NSCC is hosting the MIGSAA farewell session in applied analysis, with presentations from three current MIGSAA PhD students.

Optimal transport and nonoptimal weather

Charlie Egan • Maxwell Institute for Mathematical Sciences, Edinburgh, Scotland • C.P.Egan@sms.ed.ac.uk

Friday, 24/06/2022, 11:00-11:20 (UTC+1)

First introduced by Eady in 1949, the Eady slice equations model the formation and evolution of weather fronts. The strong discontinuities in the temperature and velocity profiles associated with weather fronts make these equations challenging to solve numerically. In this talk I will describe Cullen and Purser's 'geometric method' that was developed to overcome this issue, highlighting its relation to optimal transport, and I will discuss results from our recent implementation of this numerical method, which uses state-of-the-art techniques from the area of semi-discrete optimal transport. This is joint work with David Bourne (Heriot-Watt), Colin Cotter (Imperial), Mike Cullen (Met Office), Beatrice Pelloni (Heriot-Watt), Steve Roper (University of Glasgow) and Mark Wilkinson (Nottingham Trent).

Collective Navigation in Flowing Environments

Thomas Hodgson • Maxwell Institute for Mathematical Sciences, Edinburgh, Scotland • T.M.Hodgson@sms.ed.ac.uk

Friday, 24/06/2022, 11:20-11:40 (UTC+1)

Collective animal migrations are found across species, from the 71,000km journey of the Arctic Tern to the 44 million Red Crabs walking across Christmas Island. Despite this, the navigation methods are not well understood. In particular, marine migrations often occur in a complex flowing environment, adding difficulty to the navigation and communication for individuals. In this context, does the performance of a group depend on an animal's ability to filter out the effect of the flow on its neighbours' headings? Using a random-walk model of communication-based collective navigation, we show that more information doesn't always improve group success if individuals cannot follow others' intended headings. This is joint work with Stuart Johnston (Melbourne), Michela Ottobre (Heriot-Watt) and Kevin Painter (Torino).

Modelling the Influence of Preferential Flow and Root Architectural Traits on Drought Resistance in Plants

Andrew Mair • Maxwell Institute for Mathematical Sciences, Scotland • s1824373@ed.ac.uk

Friday, 24/06/2022, 11:40-12:00 (UTC+1)

There exists evidence to suggest that the preferential flow of water through a vegetated soil (PF) can be attributed to the architectural traits of the present plant root system. These traits, and the PF patterns they induce, may affect a plant's capacity to retain water in the soil around its roots, and hence survive periods of drought. Due to this, investigations into which root system traits induce desirable PF patterns, and improve drought resistance, are valuable to decision makers in agriculture and land management.

By modifying Richards equation we developed a novel model for water transport through soil which incorporates root-oriented PF. The finite-element method was used to obtain numerical simulations from our model equation, and we developed a Bayesian optimisation algorithm to calibrate the model against empirical data. We then used simulations from the model to assess the capacity of several root systems, which induced varying degrees of PF or exhibited different architectural traits, to mitigate water loss from the rooted zone and maximise water uptake.

When modifying the level of PF induced by a root system, our simulations revealed a trade off between water losses from evaporation and deep percolation. When keeping the level of induced PF constant, but altering architectural traits, root systems with reduced gravitropism displayed an enhanced capacity to retain water in the surrounding soil and maximise uptake efficiency.

This work shows that the architecture of root systems can be used to modify the flow of water through soil and limit losses by evaporation and deep percolation. In the future, such knowledge will help identify genotypes that are more efficient at utilising water from rainfall and irrigation.

FPS2 — Parallel Session 2

An Unsupervised Manifold Learning Approach to Untangle Big Data of Collective Human Behaviours

Fanqi Zeng • University of Bristol • fanqi.zeng@bristol.ac.uk

Friday, 24/06/2022, 11:00-11:20 (UTC+1)

Collective human behaviour such as crowd stampede in confined space is complicated to be analysed as there are plenty of nonlinear dynamics and variations. In this work, we propose using the diffusion map, an unsupervised manifold learning method, to identify the hidden patterns in collective pedestrian behaviours. We build a feature space by defining a set of measurements to extract observables from pedestrians' trajectory recordings. By applying the diffusion map on the feature spaces of one experimental data set and three simulated data sets of crowd evacuations, we then obtain the leading eigenvectors containing enriched data information. We recover the speed-density relationship from the data and distinguish different data sources based on the leading eigenvectors. We also identify the abnormal individuals without checking the original recordings. Our work contributes a convenient approach to analyse collective human behaviours trajectories without needing much prior knowledge of the data.

Clustering of Self-reported mHealth Data Trajectories

Rajenki Das • University of Manchester • rajenki.das@manchester.ac.uk

Friday, 24/06/2022, 11:20-11:40 (UTC+1)

UK based research group "Cloudy with a Chance of Pain" collected longitudinal mobile health data from the residents of the UK with chronic pain conditions to record severity of symptoms like mood, pain, sleep quality, etc. Expectation-Maximisation based clustering has been performed on the trajectories of pairs of mood and pain. We find four endotypes for the transitions happening between these pairs.

Reduced Order Modelling Using Neural Networks for Predictive Modelling of 3D-magneto-mechanical Problems with Application to Magnetic Resonance Imaging Scanners

Sayed Miah • Keele University • m.s.miah@keele.ac.uk

Friday, 24/06/2022, 11:40-12:00 (UTC+1)

The design of magnets for Magnetic Resonance Imaging (MRI) scanner requires requires multiple parameters and loading conditions to be investigated to aid with design and the manufacturing process. The coupled physical processes involved mean that a 3D magneto mechanical problem must be simulated where parameters, such as the excitation frequency and electric conductivity, are varied. Full order model simulations using finite elements require fine discretisations using dense meshes and/or high order elements and so can take up a significant amount of time and resources within the design process and, thus, can be costly. Previous work by our group has focused on the application of Proper Orthogonal Decomposition (POD) Reduced Order Models (ROM), but this has a highly invasive computational implementation. With the further coupling of additional physics in mind, alternative approached based on neural network based ROMs will be presented. In the talk, we will compare the performance of several different such ROMs for predicting the magneto-mechanical coupled simulations in both the frequency and shield conductivity parameter space using a test magnet configuration. We will conclude with some future work which include the efficient and accurate simulation of quench inside an MRI magnet with the use of machine learning for prediction.

FPS3 — Parallel Session 3

Stochastic Modelling of Agent-based Populations

Francesco Puccioni • Imperial College of London • f.puccioni20@imperial.ac.uk

Friday, 24/06/2022, 13:30-13:50 (UTC+1)

Quantifying cellular growth is crucial to understanding the dynamics of cell populations such as microbes and cancer cells. The standard behaviour of batch cultures is well known and it is usually characterised by a delay before the start of exponential growth, an exponential phase, and a steady phase; however, at the single-cell level, growth varies drastically from cell to cell due to the fluctuations in the cell cycle duration, variability caused by changing environments, and cells interactions.

At the present time, understanding how the the cell-to-cell variability affects the evolution of the entire population is still a open challenge; de facto, there are still lacking solid theoretical and simulation methods to forecast the effects of cell heterogeneity on the population dynamics.

I propose a novel stochastic model where the cells are represented by agents who divide, die, convert to other species, rejuvenate in response to an internal continuous state which increases with time.

While such models are usually only amenable to simulations, we show that the population structure can be characterized by a functional master equation which can be manipulated to obtain a novel integral renewal equation.

Compared to the classic results about renewal theory, the latter equation takes a step further. In fact, it provides a solid and compact description of the effects of cell-to-cell variability for all the populations driven by birth and death reactions.

The analytical framework allowed us to fully describe the population size distribution, population growth rate, ancestor and division times distributions. Moreover, we provide an analytical and numerical characterization of the extinction probability and first extinction times distribution for any cell-to-cell heterogeneity range. We also propose a novel way to simulate the evolution of cell populations affected by the variability of the individuals. Such computational tool allowed us to substantiate the analytical and numerical results obtained during this research project.

In conclusion, the following research project proposes a novel methodology to describe the stochastic behaviour of cell structured population with numerical, computational and analytical methods. Our results open a new theoretical path to understanding stochastic mechanisms underlying fluctuations in various biological and medical applications as: extinction of cancer cell populations under treatment, cell population growth in adverse environments and dormancy-awakening transition in breast cancer.

Exploring the Effect of Magnetic Fields on Binary Neutron Star Mergers with Numerical Hydrodynamics

Charlotte Summers • The University of Edinburgh, Scotland • charlotte.summers@ed.ac.uk

Friday, 24/06/2022, 13:50-14:10 (UTC+1)

In 2017, the Laser Interferometer Gravitational-Wave Observatory (LIGO) made the first observation of gravitational wave emission from a pair of merging neutron stars. A coincident short gamma-ray burst (GRB) provided the first direct evidence for the long-anticipated theory that these mergers could produce such electromagnetic emissions. Whilst this observation has confirmed the connection between GRBs and mergers, there are still many open questions about the mechanisms by which GRBs are produced. The theoretical complexity of mergers makes numerical fluid dynamics simulations one of the powerful tools available for investigating these questions. In this talk I will describe how numerical fluid dynamics can be used to simulate neutron star mergers, with a view to understanding the electromagnetic emissions produced by merger events. I will then present the results of neutron star merger simulations performed with the FLASH code, which investigate how the properties of the initial neutron star magnetic field affect the production of GRBs.

The Magnetic Polarizability Tensor for The Classification and Characterisation of Different Metallic Objects

James Elgy • Keele University • J.elgy@keele.ac.uk

Friday, 24/06/2022, 14:10-14:30 (UTC+1)

Low frequency metal detection is important for applications including terrorist object identification, such as knives and firearms; scrap metal sorting, archaeological surveys, and the identification of unexploded ordinance. However, current metal detectors are not able to distinguish between different shapes, small objects buried at shallow depths, and larger objects buried at greater depths. It is known that a hidden conducting object can be characterised by a complex symmetric rank 2 Magnetic Polarizability Tensor (MPT), which is a function of the object's size, shape, conductivity, permeability, and the frequency of excitation. The MPT provides an ideal object characterisation, which can be combined with a machine learning classifier. We present ongoing work concerning using finite element simulations for the classification and characterisation of small metallic objects when testing with measured MPT signatures, their validity, and the challenges associated with introducing high permeability objects.

FPS4 — Parallel Session 4

Improving the Sea State Forecast by Using the `ensembleBMA` Software and Local Wave Observations

Tatjana Kokina • University College Dublin • tatjana.kokina@ucdconnect.ie

Friday, 24/06/2022, 13:30-13:50 (UTC+1)

The main goal of this work was to establish if it is possible to improve the forecast of the sea state variables, such as significant wave height (H_s), using the forecast data available from open sources and `ensembleBMA` free software package.

In the investigation four main forecast models used by most weather agencies were used: NOAA WAVEWATCH III Global, Marine Institute (Ireland), Météo-France Wave Model (MFWAM) Global Forecast, and DWD Wave Model Global Wave Model Global. For forecast validation and training purposes real-time data was collected using a Spotter buoy, deployed just off the West Coast of Inishmaan, one of the Aran Islands in the Republic of Ireland. For part of the investigation, open data from M6 buoy (Met Eireann) was used as well.

During the study, it was established that the local forecast can be improved by at least 1% using very moderate computational power and open source data.

Authors believe that it is possible to apply this approach to a wider non-scientific population. Free access to information and the straight forward process of collecting and training the forecast opens up an opportunity to wider population to use this tool for their daily needs. This might appeal to harbour-masters, fisherman, and others who depend on the accurate sea state forecast.

High Performance Critical Line Algorithm

Josh Fogg • The University of Edinburgh, Scotland • j.fogg@ed.ac.uk

Friday, 24/06/2022, 13:50-14:10 (UTC+1)

Markowitz' Critical Line Algorithm was originally devised in the 1950s for use in finance, used to explore how to balance risk against return when creating portfolios of financial assets. Despite it's age, publicly available implementations of the algorithms have only really come to prominence over the last 20 years. My research is focused on producing a high quality, highly efficient implementation of the algorithm with further research into how these efficiency gains might allow it to be applied in other contexts.

An Efficient Adaptive Collocation Method for Approximating Parabolic PDEs with Random Data

Benjamin Kent • University of Manchester • benjamin.kent@manchester.ac.uk

Friday, 24/06/2022, 14:10-14:30 (UTC+1)

In this talk, we discuss an adaptive method to efficiently approximate the solution to parametric, parabolic partial differential equations. We discretise the problem in a non-intrusive manner using stochastic collocation, timestepping and finite element methods. Adaptivity is driven by an a posteriori error estimation strategy that estimates the distinct contributions to the total approximation error stemming from both the parametric and timestepping discretisation.

Numerical results will be presented for the time-dependent advection diffusion problem with an uncertain advective field. The evolution of error in time and the challenges of forming an adaptive in time approximation are discussed.

Contributed Poster Session

Adaptive Stabilised Mixed Finite Element Method Combined with the Method of Characteristics for a Stationary Convection-diffusion-reaction Problem

Mary Chriselda Antony Oliver • University of Leeds • chriseldaoliver23@gmail.com

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

We consider a stationary convection-diffusion-reaction problem in two or three-dimensional bounded domains. We approximate this model by a non-stationary problem and propose a numerical method which combines the method of characteristics with a mixed finite element procedure. In order to avoid any compatibility condition between the discrete spaces, we propose an augmented scheme and show it has a unique solution. We also derive a residual-based a posteriori error indicator and show it is reliable and locally efficient. Finally, we provide some numerical experiments that illustrate the performance of the corresponding adaptive algorithm.

CLASSIX: Fast and Explainable Clustering Based on Sorting

Xinye Chen • The University of Manchester • xinye.chen@postgrad.manchester.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

We introduce a fast and explainable clustering method called CLASSIX, which shares features of both distance and density based clustering methods. It consists of two phases, namely a greedy aggregation phase of the sorted data into groups of nearby data points, followed by the merging of groups into clusters. The algorithm is controlled by two main parameters, namely a distance parameter for the aggregation and another parameter controlling the minimal cluster size. The algorithm has linear space complexity and achieves near linear time complexity on a wide range of problems. Its inherent simplicity allows for the generation of intuitive explanations of the computed clusters. The software and experimental data are publicly available at https://github.com/nla-group/classix .

Spending Energy for a Reward: Understanding the Fine Movements of Badgers

Jessica Furber • University of Surrey • j.furber@surrey.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

The purpose of the current study is to establish a modelling framework to understand the movement of the European badger (Meles meles) within their environment. It is widely understood that badgers play a crucial role in the transmission of bovine Tuberculosis (bTB), but it is still not clear on how this role is played. An approach to modelling animal movement is using energy potentials and stochasticity, primarily seen in physics to describe particle motion. Such approach has been successful in describing the movements of free ranging Mountain elk (Cervus elaphus) and their avoidance to vehicles and humans but has yet to be applied within the badger community.

A modelling framework has been built that describes how badgers move around their landscape trying to forage, defecate, interact with other badgers (including male and female differences). The model incorporates general badger behaviour, badger social interaction, and random walk/individual behaviour. We use data driven methods to parametrize the model using GPS data and interpret the level of noise within the system.

Key questions this modelling framework will allow us to answer are: What is the effect of removing a single dominant badger? How does the climate affect badger movement? How does badger movement affect the spread of bTB? The answer to these questions could be crucial in the role of strategy planning and more.

In this poster, we present preliminary results on the fitted/parameterized model and explore some of the key modelling questions.

Improving Power by Conditioning in Genetic Association Studies (GWAS)

Mahfuzur Rahman Khokan • The Open University • mahfuzur.khokan@open.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

In the area of statistical genetics, classical genome-wide association studies (GWAS) assess the association between a biological characteristic and genetic variants, working with one variant at a time in a regression model, and reporting the most significant associations. However, in many cases there are known databases of major genetic variants that have a substantial effect on the trait. In such situations it makes sense statistically to condition on these major variants to improve power in detecting associations with new variants; but this is not a common practice in GWAS applications.

In this study, we show theoretically and computationally how conducting a joint analysis of the genetic variants in a multivariate regression model, where the estimated effects of a new variant is conditioned upon some major variants, can improve the performance of the model in terms of reducing the standard error and improving the power. The amount of gain of power will depend on the correlation between the response and the covariates, as well as correlation between the covariates. We further show that conditional results can sometimes be obtained from publicly available summary statistics reported for univariate associations in published GWAS studies, even when the individual-level data are unavailable.

A prominent example of such a trait is skin colour, for which there are many studies consistently identifying a handful of major genes. We will look into a dataset for over 6,500 mixed ethnicity Latin Americans to see how the conditioning process can improve the detection power of GWAS studies and identify new genetic variants in such a situation.

Onset of Chaos in the Pythagorean Three-body Problem

Mika Kontiainen • The University of Edinburgh, Scotland • mikakonte99@gmail.com

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

The three-body problem has tormented physicists and mathematicians alike since Newton first formulated his theory of gravity in the late 17th century. Due to its chaotic nature, the problem eludes analytic solution and numerical methods are required. While modern computational capabilities have made a statistical description of the end states possible, the physical origin of chaos and transitions observed in the rate of divergence between two solutions are less well understood. Taking the Pythagorean formulation of the problem as our starting point, we present preliminary numerical results regarding these aspects of the problem, tying orbital geometry and complexity together.

Information Measures Estimation and Random Projection

Haoran Ni • University of Warwick • haoran.ni@warwick.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

The Mutual Information (MI) between two random variables measures the reduction in uncertainty of one random quantity due to information obtained from the other. It is an important information-theoretic concept, closely related to Entropy, that plays a role in many applications, including decision trees in machine learning, independent component analysis (ICA), gene detection and expression, link prediction, topic discovery, image registration, feature selection and transformations, and channel capacity.

A persistent challenge is the accurate numerical estimation of mutual information from high-dimensional data, a problem arising in image classification, microarray data analysis, and machine learning. For example, in machine learning the mutual information is used to regularize Generative Adversarial Networks (GANs) in order to produce samples of high-dimensional data with greater diversity.

The proposed research project aims to develop new and efficient mutual information estimation systems that produce accurate results irrespective of sample size, dimensionality, and correlation. Among other methods, the approach is based on fast and sparse Johnson-Lindenstrauss transforms in order to reduce the dimension of the data, an approach that has proven to be successful in compressed sensing, algorithms for streaming data, and topological data analysis. The main expected benefit is a computational complexity that depends on the amount of data and on the intrinsic complexity of the data, rather than the ambient dimension, leading to substantial savings in time and potentially space. An example of intrinsic complexity is provided by image data, where images are presented by a certain number of pixels (for example, 1024×1024), but image compression methods based on the Fourier or Wavelet transforms show that a typical image can be represented using far less information. Ideally, we want algorithm operating on such images to depend on the amount of information necessary to encode the image, rather than the “visible” dimension.

Convergence of Deep Gaussian Processes

Conor Osborne • Maxwell Institute for Mathematical Sciences, Scotland • conor.osborne@ed.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

Gaussian processes have proved to be a powerful and flexible tool in the reconstruction of functions given a set of known data points, with applications in machine learning, optimisation and data assimilation. However, they can be limited when the functions being reconstructed are of a non-stationary or anisotropic nature. Deep Gaussian processes, constructed using a hierarchical process where the inputs to a Gaussian process are themselves Gaussian processes, aim to give a more flexible approach to function reconstruction.

We look at convergence rates of these deep Gaussian processes in terms of the number of known data points. We also show that deep Gaussian process regression achieves considerably better results than standard Gaussian process regression when reconstructing non-stationary and anisotropic functions.

Impact of Covid-19 on Oil prices Volatility and their Recovery

Nida Siddiqui • Heriot-Watt University • ns2026@hw.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

In financial markets, volatility is a statistical measure of the dispersion of re- turns around the mean price. The most widely used measure of financial risk is volatility. Crude oil prices play a crucial role in world economics and a high level of volatility in these prices directly impacts the economic stability of importing and exporting nations. Covid-19 has had a major impact on oil prices around the world. In this research we model and forecast crude oil prices volatility of the cash prices of Das Blend UAE, which is a blend of one of the worlds bench- mark crudes, Dubai Crude. The research aims to estimate the time it will take for the oil prices to recover from the shock of Covid-19 and reach their historical peak in the absence of any other shocks. The data covers a time period of two years starting from the 1st of January, 2018 till 31st January, 2022. Time series analysis is a very reliable approach for modelling and forecasting volatility. Traditional time series models assume a normal distribution of returns, and hence constant variance of the error terms. But empirical data for crude oil prices does not support this assumption. The returns are not normally distributed (leptokurtic) and hence variance is not constant, instead it keeps on evolving. In this research, we use the GARCH model and its variations from time series, to capture the non-constant variance and produce formidable forecasts. The analysis was carried out using the R studio package, `rugarch`, which is an R package for univariate GARCH models. Several GARCH models are analysed assuming normal distribution as well as Student t distribution of errors. The AIC and BIC criteria are used to choose the best t model. Applying simulation techniques to the selected model, we try to work out the probabilities of the crude oil prices reaching their historical peak.

Novel Analysis Methods to Process Fluorescence Imaging Data and Characterise Epileptic Paroxysms

Adam Smith • University of Warwick • adam.smith.1@warwick.ac.uk

Thursday, 24/06/2022, 17:00-18:30 (UTC+1)

Electrophysiological techniques are commonly used methods to investigate neuronal dynamics. However, these methods suffer from limited spatial resolution. Wide-field fluorescent calcium imaging can overcome these limitations by facilitating the optical readout of local neuronal activity with a high spatial resolution. Our research focuses on using these tools to characterise the interactions between spreading paroxysmal events, such as seizure and spreading depolarization, across a large area of the cortical surface. Analysing such data through manual methods is challenging and often not feasible given the number of pixels one would have to process. Previous studies have analysed these methods by empirical observation or reductive discrete region-of-interest selection. Here, we develop a comprehensive, semi-automated Python-based analysis pipeline, to allow characterisation of these events across the entire field-of-view. To successfully develop these analytical tools, we first characterise a novel method of spike detection with its robustness owed to the spatial extent of the data. We utilise these spikes as a reference point for the target phenomena. The novel measure of inter-spike-recovery levels is sufficient to define seizure states and other prolonged periods of a sustained increased calcium marked spreading depolarization states. The result includes the ability to continuously track seizure and SD propagation across our entire field-of-view, and to characterise their interaction with underlying brain network activity. Due to the novelty of these techniques, and the occurrence of these paroxysms in many disease states, the developed tools hold great promise in assisting the wider neuroscience community in unravelling the complex neuronal dynamics in multiple pathological environments. We envision these tools will provide novel insight into seizure-SD interactions and guide future mathematical studies to support patterns in experimental data in epilepsy.

Participants NSCC

Edinburgh 2022

Plenarists

Andrew Duncan (p6)

Gabriela Gomes (p5)

Martin Schmidt (p5)

Małgorzata Zimoń (p6)

Organisers

Jonna Roden [Chair]

Matthew Holden

Savvas Melidonis

Andrés Miniguano-Trujillo

Speakers - Contributed talks

Ivet Galabova (p8)

Xell Brunet Guasch (p10)

Enda Carroll (p15)

Rajenki Das (p19)

Charlie Egan (p17)

James Elgy (p22)

Josh Fogg (p24)

Monserrat Guedes Ayala (p9)

Muhammad Mahmudul Hasan (p13)

Thomas Hodgson (p18)

Oscar Holroyd (p16)

Benjamin Kent (p24)

Tatjana Kokina (p23)

Andrew Mair (p18)

Sayed Miah (p20)

Jenny Power (p11)

Farhana Akond Pramy (p15)

Francesco Puccioni (p21)

Prerna Singh (p12)

Charlotte Summers (p22)

Yu Tian (p14)

Huining Yang (p14)

Filippo Zanetti (p9)

Fanqi Zeng (p19)

Speakers - Poster session

Mary Chriselda Antony Oliver (p26)

Xinye Chen (p26)

Jessica Furber (p26)

Mahfuzur Rahman Khokan (p27)

Mika Kontiainen (p27)

Haoran Ni (p28)

Conor Osborne (p28)

Nida Siddiqui (p29)

Adam Smith (p29)

Attendants

Maryam Alarfaj

Adam Aldridge

Miguel Anjos

Karolina Benková

Rebecca Brady

Andrew Cleary

Edward Dolon

Anastasia Istratuca

Johanna Järvsoo

Panagiotis Kaklamanos

Teresa Klatzer

Siyuan Ma

Ibrahim Mohammed

Keila Moral

Obed Nwachukwu

Bárbara Rodrigues

Nagisa Sugishita

Aidan Tully

Simon Urbainczyk

Swetha Usha Lal

Peter Whalley

Minhui Zhou

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