### British Applied Mathematics Colloquium 2019

#### Conference Agenda

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<td><strong>9:00am - 9:50am</strong></td>
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<td><strong>Session Chair: Jonathan Dawes</strong></td>
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<td><strong>Jessica G Williams, Sarah L Waters, Derek E Moulton, Ben W Turney</strong></td>
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<td><strong>Mathematical Institute, University Of Oxford, United Kingdom</strong></td>
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<td><strong>Matthew Allan Nethercote¹, Raphael Assier², Ian David Abrahams³</strong></td>
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<td>¹University of Manchester, United Kingdom; ²University of Manchester, United Kingdom; ³University of Cambridge, United Kingdom</td>
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Cancer is a complex disease that starts with mutations of key genes in one cell or a small group of cells at a primary site in the body. If these cancer cells continue to grow successfully and, at some later stage, invade the surrounding tissue and acquire a vascular network, they can spread to distant secondary sites in the body. This process, known as metastatic spread, is responsible for around 90% of deaths from cancer and is one of the so-called hallmarks of cancer.

To shed light on the metastatic process, we present a mathematical modelling framework that captures for the first time the interconnected processes of invasion and metastatic spread of individual cancer cells in a spatially explicit manner – a grid, hybrid, individual-based approach. This framework accounts for the spatiotemporal evolution of mesenchymal- and epithelial-like cancer cells, membrane-type-1 matrix metalloproteinase (MT1-MMP) and the diffusible matrix metalloproteinase-2 (MMP-2), and for their interactions with the extracellular matrix.

Using computational simulations, we demonstrate that our model captures all the key steps of the invasion-metastasis cascade, i.e., invasion by both heterogeneous cancer cell clusters and by single mesenchymal-like cancer cells; intravasation of these clusters and single cells both via active mechanisms mediated by matrix-degrading enzymes (MDEs) and via passive shedding; circulation of cancer cell clusters and single cancer cells in the vasculature with the associated risk of cell death and disaggregation of clusters; extravasation of clusters and single cells; and metastatic growth at distant secondary sites in the body. By faithfully reproducing experimental results, our simulations support the evidence-based hypothesis that the membrane-bound MT1-MMP is the main driver of invasive spread rather than diffusible MDEs like MMP-2.

The mathematical analysis and numerical simulation of acoustic and electromagnetic wave scattering by planar screens is a classical topic. The standard technique involves reformulating the problem as a boundary integral equation on the screen, which can be solved numerically using a boundary element method. Theory and computation are both well-developed for the case where the screen is an open subset of the plane with smooth (e.g. Lipschitz or smoother) boundary. In this talk I will explore the case where the screen is an arbitrary subset of the plane; in particular, the screen could have fractal boundary, or itself be a fractal. Such problems are of interest in the study of fractal antennas in electrical engineering, light scattering by snowflakes/ice crystals in atmospheric physics, and in certain diffraction problems in laser optics. The roughness of the screen presents challenging questions concerning how boundary conditions should be enforced, and the appropriate function space setting. But progress is possible and there is interesting behaviour to be discovered: for example, a sound-soft screen with zero area (planar measure zero) can scatter waves provided the fractal dimension of the set is large enough. Accurate computations are also challenging because of the need to adapt the mesh to the fine structure of the fractal. As well as presenting numerical results, I will outline some of our recent theoretical results, and some outstanding open questions, from the point of view of numerical analysis of boundary element method approximations.

The problem of interest is that of a whispering gallery high-frequency asymptotic mode propagating along a concave part of a boundary and approaching a boundary inflection point. Like Airy ODEs and associated Airy function are fundamental for describing transition from oscillatory to exponentially decaying asymptotic behaviours and so e.g. transition from light to shadow near caustics at high frequencies, the boundary inflection problem leads to an arguably equally fundamental canonical boundary-value problem for a special PDE, describing transition from a “modal” to a “scattered” asymptotic behaviour. The latter problem was first formulated and analysed by M.M. Popov starting from 1970s [1]. The associated solutions have asymptotic behaviours of a modal type (hence with a discrete spectrum) at one end and of a scattering type (with a continuous spectrum) at the other end. Of central interest is to find the map connecting the above two asymptotic regimes. The problem however lacks separation of variables, except in an asymptotical sense at
both of the above ends, and has over the years proved not to be explicitly solvable. Nevertheless, certain progress can be made by its asymptotic analysis as well as subsequent numerical analysis.

The presentation will review the background, and will present some recent progress, e.g. [2]. In particular, a perturbation analysis of the problem at the continuous spectrum end, as well as the fact that the solutions remain exponentially decaying sufficiently far away from the boundary, allow to deform the integrals over the continuous spectrum into the complex plane. The values of the analytic continuation of a limit spectral function at certain points appear to describe the intensities of creeping waves emerging behind the inflection point, and ultimately the desired map connecting the two asymptotics. The evaluation of the actual “scattering matrix” may be quite a delicate numerical problem, and we will discuss certain ways in that direction including re-formulation of the problem as a one-dimensional boundary integral equation and its further regularization.


11:30am - 1:00pm
Minisymposium 2A: Nonlinear dispersive waves
Session Chair: Karima Khusnutdinova
Session Chair: Emilian I. Parau

11:30am - 12:00pm
Hydroelastic waves over constant vorticity flows: solitary waves and modulational instabilities
Paul Milewski¹, Tao Gao¹, Zhan Wang²
¹University of Bath, United Kingdom; ²Chinese Academy of Sciences

The problem of waves in constant vorticity flows under a surface plate that resists flexion is studied using modulational theory. Various envelope models are derived (including the nonlinear Schrodinger equation). Using these models as guidance for the expected behaviour of the fully nonlinear Euler equations with the flexible plate, we find branches of solitary waves and explore the stability of Stokes waves. An example of a flow that could be modelled this way is Couette flow under a flexible ice sheet, and we comment on applicability and criteria for ice fracture.

12:00pm - 12:30pm
Application of the non-local AFM method in cylindrical geometry
Emilian I. Parau
University of East Anglia, United Kingdom

The AFM (Ablowitz-Fokas-Musslimani) method applicable to studying water waves is extended to a cylindrical geometry. The formulation involves only surface variables. The method is developed for a general cylindrical surface, and we use it for computing fully nonlinear axisymmetric periodic and solitary waves on a ferrofluid column. This is joint work with Mark Blyth(UEA).

12:30pm - 1:00pm
Nonlinear Hydroelastic Waves
Jean-Marc Vanden-Broeck
University College London, United Kingdom

Nonlinear waves propagating under an elastic sheet are considered. Such waves can be viewed as a model for waves propagating under an ice sheet. Various numerical procedures are reviewed. New results for symmetric and non symmetric waves are presented.

11:30am - 1:00pm
Minisymposium 3A: Network dynamical systems in mechanics and biology.
Session Chair: Alexander Erlich
Session Chair: Andrew L. Krause

11:30am - 12:00pm
Metapopulation Models in Ecology & Epidemiology
Andrew L. Krause¹, Robert A. Van Gorder², Nabil Fadai³
¹University of Oxford, United Kingdom; ²University of Otago, New Zealand; ³Queensland University of Technology, Australia

Metapopulation models represent spatially-distributed populations by associating a distinct population with each node, and allowing for immigration or other contacts via edges, with dispersal from a population determined via local connectivity. Here we present results on two examples of such models, highlighting open challenges. The first is a model of predation involving delayed dispersal, where immigration of a predator between populations is not instantaneous. Analyzing the resulting delay differential equations demonstrates that this time delay can both regularize and destabilize the overall population dynamics, both in the case of coexistence steady states, and in more complicated behaviours such as chaotic dynamics. Finally we discuss stochastic infections in an SIS model on a network, and discuss open challenges in controlling disease dynamics in the presence of uncertainty.

12:00pm - 12:30pm
Mechanical Characterisation of Disordered and Anisotropic Cellular Monolayers
Alexander Nestor-Bergmann¹, Emma Johns², Sarah Woolner³, Oliver Eskild Jensen²
¹University of Cambridge, United Kingdom; ²University of Manchester, United Kingdom;
Characterising the mechanical properties of geometrically complex tissues is an essential step in understanding how cell behaviours can be controlled by mechanical cues. Working in the context of a popular vertex-based model, I will provide expressions for the linearised relation between tissue-level stress and strain about a deformed base state, showing that mechanically homogenised tissues can exhibit anisotropic mechanical properties. The model captures observations of an epithelium from a Xenopus embryo, where uniaxial stretching induces spatial ordering, with cells under net tension (compression) tending to align with (against) the direction of stretch, but with the stress remaining heterogeneous at the single-cell level. Expressions for the elastic tissue moduli can be written as direct sums over cells, predicting that tissue properties can be tuned to a regime with high elastic shear resistance but low resistance to area changes, or vice versa.

12:00pm - 1:00pm

**Autonomous actuation of active mechanical networks**

Francis Woodhouse  
University of Oxford

Unlike the air around us, biological systems are not in equilibrium: cells consume chemical energy to keep growing and moving, forming a clear arrow of time. The recent creation of artificial versions of these ‘active’ systems raises the tantalising prospect of soft robotic systems fuelled by as simple a source as oxygen. After an introduction to the physics of natural and artificial active systems, we will see how endowing mechanical networks with activity can create intricate self-actuating mechanisms.

11:30am - 1:00pm  
**Contributed Talks 13: Epidemiology and ecology**  
Session Chair: Sandro Azaele

11:30am - 11:50am

**Incorporation of Awareness Programs into a Model of the Spread of HIV/AIDS amongst People who Inject Drugs (PWIDs)**

Maha ALSHARARI  
University of Strathclyde, United Kingdom

Mathematical modelling techniques have been used extensively during the HIV epidemic. Injecting drug use is an increasing cause of HIV transmission in most countries worldwide. The media plays an important role in spreading health awareness by changing mixing behaviour. The published studies show some of the mathematical models which have been used to explore the effect of media awareness programs on the spread and control of infectious disease (1). In this talk, we have developed a mathematical model of the effect of disease awareness programs on the prevalence of HIV amongst people who inject drugs (PWIDs), building on the models developed by (2) and (3). A system of differential equations has been deduced to describe the improved model that reduces the spread of the diseases through the effect of awareness of disease on sharing needles and syringes amongst the PWID population. The model supposes that PWIDs clean their needles before use rather than after. We perform an equilibrium and stability analysis for this model. Our discussion has been focused on two ways of studying the effect of awareness programs in disease transmission models. The key biological parameter of our model is the basic reproductive number $R_0$. We find that there is a critical threshold parameter $R_0 = 1$ which determines the behaviour of the model. We have shown that the system has a unique equilibrium solution, then we have shown that if $R_0 \leq 1$ then the disease-free equilibrium is globally asymptotically stable, so whatever the initial fraction of infected individuals the disease will die out as time becomes large. If there is no disease initially present then there will never be any disease. If $R_0 > 1$ then there is the disease-free equilibrium and additionally a unique endemic equilibrium. If there is disease initially present and $R_0 > 1$ then the system tends to the unique endemic equilibrium. We also showed that the disease-free equilibrium is locally asymptotically stable if $R_0 < 1$, neutrally stable if $R_0 = 1$ and unstable if $R_0 > 1$. In the case that $R_0 > 1$ we showed that the endemic equilibrium was locally asymptotically stable too. Our analytical results are confirmed by using simulation with realistic parameters values. A brief summary concludes the talk.

11:50am - 12:10pm

**Anticipating Disease Elimination**

Emma Southall$^1$, Adjani Dessavre$^1$, Michael Tildesley$^{1,2}$, Louise Dyson$^{1,2}$  
$^1$Mathematics institute, University of Warwick, UK; $^2$School of Life Science, University of Warwick, UK

A challenging problem in infectious disease modelling is assessing when a disease has been eliminated. If campaigns are stopped prematurely it can result in disease resurgence and subsequently put control efforts back by decades. This talk presents potential indicators of elimination detected in spatially collected timeseries data. Bifurcations in a system can be predicted prior to reaching the dynamical threshold. Our research shows that an infectious disease system will undergo the phenomenon of Critical Slowing Down when it crosses through the critical transition to elimination. Critical Slowing Down theory predicts that perturbations away from the steady state will recover more slowly as the system approaches the bifurcation. Statistical indicators of Critical Slowing Down have been detected in timeseries data of many dynamical systems from climate, to ecosystems and financial markets. A challenge when detecting critical transitions is that of accurately ‘detrending’ the signal, in order to preserve the statistical properties of the fluctuations. A metapopulation is a network of interacting populations where the infection dynamics are influenced by events within populations and by spatial processes between connected populations. This talk will present using a metapopulation framework to investigate disease elimination by detrending the signal using information from the other subpopulations.
The waving motion of human sperm flagella is the archetype of spatiotemporal self-organization in nature and critical for reproduction. Flagellar waves result from the combined action of hundreds of molecular motors deeply embedded in the flagellar structure that bend, shear and twist the flagellum in three-dimensions to generate a helical propulsion. Nevertheless, our understanding of the flagellar movement has been limited thus far to microscope planar projections. Here we employ a state-of-the-art, high-speed 3D microscope imaging capture with bespoke mathematical imaging processing capable of resolving the flagellar movement in 4D (3D+time) with high-resolution. This allows novel exploration of the flagellar kinematics in 3D, from simple head trajectories to curvature and torsion with a microscopic resolution. This revealed a novel complex regulatory mechanism coupling bending and torsional travelling waves. We observe for the first time that kinematic torsion is singularly distributed along the flagellum, and capable of inducing a novel flagellar helical ‘perversion’ phenomenon. The latter is found in helices composed by sections of opposite chirality. Such flagellar perversion is however dynamical, and travels during the beat. As a result, the chirality of the flagellum, that is the handiness of the helical waveform, is not conserved along the flagellum. We further show that this phenomenon may lead to artefacts on the curvature waves if examined with a 2D microscope. The lack of conserved chirality of the flagellar waveform may stabilise the sperm ascension in convoluted flows and geometry within the reproductive tract.
Morphogenetic movements in epithelial tissues require tight spatiotemporal control over cell-cell junction lengths. Contractile forces alter cell contact lengths in a cyclic fashion as a mechanical ratchet. Here, pulses of actomyosin actomyosin accumulation are thought to drive ratcheting through acute periods of junctional contraction. Using optogenetic control of actomyosin contraction, we find that epithelial junctions show elastic behaviour under low stress, returning to their original length after contraction, but show irreversible deformation under high contractile stress. Using the classical vertex model for epithelium, we are unable to capture these results, with junctions displaying either only elastic or only viscous behaviour, depending on the choice of mechanical parameters. We thus developed a new model for adaptive junctional length regulation via strain-sensitive remodelling of junctional tension. This model is able to capture the viscoelastic behaviour of the epithelial junctions in line with experiments, and predicts robust mechanical ratcheting under repeated junctional contractions.

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**Bridging the gap between individual-based and continuum models of growing cell populations**

**Fiona Macfarlane**

University of St Andrews, United Kingdom

Continuum models for the spatial dynamics of growing cell populations have been widely used to investigate the mechanisms underpinning tissue development and tumour invasion. These models consist of nonlinear partial differential equations that describe the evolution of cellular densities in response to pressure gradients generated by population growth. Little prior work has explored the relationship between such continuum models and related single-cell-based models. We present here a simple stochastic individual-based model for the spatial dynamics of multicellular systems whereby cells undergo pressure-driven movement and pressure-dependent proliferation. We show that nonlinear partial differential equations commonly used to model the spatial dynamics of growing cell populations can be formally derived from the branching random walk that underlies our discrete model. Moreover, we carry out a systematic comparison between the individual-based model and its continuum counterparts, both in the case of one single cell population and in the case of multiple cell populations with different biophysical properties. The outcomes of our comparative study demonstrate that the results of computational simulations of the individual-based model faithfully mirror the qualitative and quantitative properties of the solutions to the corresponding nonlinear partial differential equations. Ultimately, these results illustrate how the simple rules governing the dynamics of single cells in our individual-based model can lead to the emergence of complex spatial patterns of population growth observed in continuum models.

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**Computational modelling and simulation of cancer growth and migration within a 3D heterogeneous tissue**

**Cicely K. Macnamara, Alfonso Caiazzo, Ignacio Ramis-Conde, Mark A.J. Chaplain**

1. University of St Andrews, United Kingdom; 2. Weierstrass Institute for Applied Analysis and Stochastics (WIAS); 3. Universidad de Castilla la Mancha, Departamento de Matematicas

The term cancer covers a multitude of bodily diseases, broadly categorised by having cells which do not behave normally. Since cancer cells can arise from any type of cell in the body, cancers can grow in or around any tissue or organ making the disease highly complex. One of the main Hallmarks of Cancer (Hanahan & Weinberg, 2000; 2011) is tissue invasion and metastasis. Mathematical modelling and simulation can complement traditional biological and experimental approaches to cancer research. Our research is focused on understanding the specific mechanisms that occur in the tumour microenvironment. We are developing a novel model which allows one to simulate the behaviour of and spatio-temporal interactions between cells, blood vessels and other components of the tumour microenvironment. We use a 3D individual-based force-based model, i.e. each element (a single cell, for example) is fully realised within the model and interactions are primarily governed by mechanical forces between elements. In this way we are able to reproduce, in silico, complex features of tumour development such as growth around a blood-vessel network or along the striations of fibrous tissue. As well as the mechanical interactions we also consider chemical interactions. For example, by coupling the code to a finite element solver to model the diffusion of oxygen from blood vessels to cells. In this talk I will present the current state of the art of the model and its capabilities.

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**Discrete-to-continuum modelling of cells to tissue**

**Nicholas A. Hill, Roxanna G. Barry, Peter S. Stewart**

University of Glasgow, United Kingdom

We consider a single line of nonlinearly hyperelastic cells of finite size, with forces transmitted across the boundaries between neighbours. One or both ends of the line are fixed to represent free expansion or confinement. The dynamics of the array is given by a system of discrete 1D ODE's. Individual cells grow in volume and divide into two identical daughter cells. The parent cell divides its mass equally so that each daughter cell is half the total length of the parent cell, and an extra boundary at the midpoint of the parent cell is introduced. Two examples of resistance to motion are considered. Firstly, we suppose that the cells are able to reproduce, although a stochastic individual is able to reproduce, highly complex. One of the main Hallmarks of Cancer (Hanahan & Weinberg, 2000; 2011) is tissue invasion and metastasis. Mathematical modelling and simulation can complement traditional biological and experimental approaches to cancer research. Our research is focused on understanding the specific mechanisms that occur in the tumour microenvironment. We are developing a novel model which allows one to simulate the behaviour of and spatio-temporal interactions between cells, blood vessels and other components of the tumour microenvironment. We use a 3D individual-based force-based model, i.e. each element (a single cell, for example) is fully realised within the model and interactions are primarily governed by mechanical forces between elements. In this way we are able to reproduce, in silico, complex features of tumour development such as growth around a blood-vessel network or along the striations of fibrous tissue. As well as the mechanical interactions we also consider chemical interactions. For example, by coupling the code to a finite element solver to model the diffusion of oxygen from blood vessels to cells. In this talk I will present the current state of the art of the model and its capabilities.
the motion of a cell boundary relative to its neighbours so that the damping force is proportional to the rate of elongation of the cell (Kelvin dissipation). Having constructed and solved the discrete model, we then use the methods of discrete-to-continuum upscaling to derive new PDE models using Taylor expansions local to each discrete cell, which requires that the properties of the individual cells (e.g. shear modulus) vary smoothly along the array. The discrete and PDE models are solved computationally for a range of imposed boundary and growth conditions. We demonstrate excellent agreement between the solutions (including diagnostics such as pressure and stretch along the array) of the discrete and PDE models for a number of examples, including a ring of cells (e.g. myocytes) with a wave of active contraction, growth of incompressible neo-Hookean cells, and stress-dependent growth. Qualitative differences are found in long-time scaling laws for the growth of the array of cells for stress-dependent and independent cell division rules.

12:30pm - 12:50pm

A mathematical model for photothermal ablation of spherical tumors

Ahmed Mostafa Abdelhady Ismaeel
Uni of Glasgow, United Kingdom

Photothermal ablation is a promising new technique for treatment of some cancers, where metal nanoparticles are introduced into the tumour and the system is locally heated with a laser to destroy the malignant cells. The aim is to have nanoparticles accumulate within the tumour and not in the surrounding healthy tissue, so that the heat source leads to a differential increase in temperature in the cancer and hence cell death. In this study we consider a mathematical model for nanoparticle delivery to a vascularised spherical tumour, examining the distribution of nanoparticles through the tumor and the surrounding tissue. In this model we consider nanoparticles conjugated with ligands which selectively bind to tumor cell surface receptors and eventually leads to nanoparticle internalization within the cell. We study how the mass of accumulated nanoparticles within the tumor (and the surrounding tissue) is influenced by the degree of tumour vascularity, ligand nanoparticle conjugation and tumor cell capacity for internalized nanoparticles. We validate our model predictions against experimental data in vivo. We suggest an optimal timescale to maximize the efficiency of ablation across a range of physiological cases.

11:30am - 1:00pm

Contributed Talks 26: Industrial modelling 1
Session Chair: Matthew Haynes

11:30am - 11:50am

Mathematical Modelling of Metal Forming

Hanson Bharth
University of Warwick, United Kingdom

This talk explores the mathematical modelling of a metal sheet deformed by a rigid roller, by considering a model of an elastic half-space and a rigid roller. Analysing the indentation of the elastic half-space by the rigid cylindrical roller, subject to a stick-slip model of friction, gives rise to a matrix Wiener-Hopf problem which is due to the interaction points (stick-slip junctions).

11:50am - 12:10pm

Multiscale Modelling Methods for the Flow During Grinding

Zakhary Crowson, John Billingham, Paul Houston
University of Nottingham, United Kingdom

During the machining process of grinding, large temperatures are generated in the cutting zone which demands the application of a fluid in order to regulate the heat load: this fluid acts as both a lubricant and a coolant for the process. Mathematically understanding the dynamics of the flow is vital in optimising this fluid delivery during grinding, especially given the numerous difficulties presented in experimentally investigating this flow.

While numerical solutions to this turbulent, multiphase flow are both computationally demanding and difficult to obtain over the whole flow domain, distinct flow regions exist where the physics of the flow vary dramatically. In this work, we use asymptotic methods to show how the flow domain can be separated into a micrometre-scale inner domain and a centimetre-scale outer domain, with the focus being on the inner region. In this region, we look to reduce the problem by applying the lubrication approximation, which is followed up by then looking at the two-scale homogenisation of the system. The manifestation of the infamous moving contact line problem in this system is discussed before solutions to these systems, obtained with a combination of finite-element and finite-difference methods, are presented.

12:10pm - 12:30pm

Exact solutions of the Laplace-Young equation in parametric form for a horizontal liquid bridge

Kevin Martin Moroney, Matthew Haynes, Stephen B. G. O'Brien
University of Limerick, Ireland

In this work, we consider the shape of a horizontal liquid bridge suspended between two vertical walls. The study is motivated by the desire to study the stability of liquid bridges formed in the coating process of tubular meshes making up a stent. The tubular mesh is constructed of superalloy wires with a repeating diamond structure, which supports liquid bridges of coating material. As the coating material is cured solvent evaporates, causing a drop in bridge volume, which sometimes resulting in hole formation. The minimum volume of a stable bridge is of interest. Preliminary investigation considers the determination of the shape of a horizontal two dimensional fluid bridge fixed between vertical walls. Previous work has considered asymptotic solutions to a parametric formulation of the Laplace-Young equation [1]. Here, we consider the
exact solution to this parametric formulation using elliptic integrals. The solutions are derived and analysed. Solutions to the parametric equations alone will permit cases which are not physically feasible, such as intersecting upper and lower bridge surfaces. Thus extra physical constraints on the solutions are considered. The exact solutions are compared to numerical solutions of the problem. The solutions are also compared to asymptotic solutions for small Bond numbers derived in [1].

References

12:30pm - 12:50pm

**Flexure Coupling Mechanisms for High Performance Robotics and Automated Processes**

**Jianhang Ding, Nicola Bailey, Patrick Keogh**

University of Bath, United Kingdom

Currently robotics and automated machinery adopt mechanical structures which containing hinges, bearings and other complex joints. However, these joints cause wear and have backlash, friction and compliance, which leads to the motion precision on a small scale to not be satisfying. Flexure couplings, which are pseudo-joints that utilise the elastic properties of a material, can eliminate these tribological effects. Therefore, replacing the conventional multibody systems joints with flexure couplings can improve the precision movement of the system.

This work focusses on the deformation of a single flexure coupling when applying a load. A model is derived within is based on Euler-Bernoulli large deflection beam theory, and results in a system of first order differential equations. A compound compliant joint, which combines two or more flexure couplings clamped together at both ends, is also examined and the model becomes more difficult. A detailed study concentrates on a parallel link compliant joint where the solution is based on a lsqnonlin optimisation scheme. A stepping algorithm is used so the deflection of the parallel link compliant joint can be found, dividing the forces by a large number and applying the small force at the end of the coupling gradually. The algorithm works well when the couplings are not significantly close.

11:30am - 1:00pm

**Contributed Talks 33: Porous media and flow networks**

**Session Chair: Alexandra Tzella**

11:30am - 11:50am

**Axisymmetric flow in a heterogeneous aquifer**

**Edward Hinton, Andrew Woods**

University of Cambridge, United Kingdom

We study the flow that arises when a relatively buoyant fluid is injected at a constant rate into a confined, axisymmetric porous medium originally saturated with a second fluid of different density and viscosity. We investigate the effect of permeability that varies vertically within the aquifer. We derive a PDE for the evolution of the interface between the two fluids, which identifies that the evolution is self-similar at all times with the radial extent growing in proportion to \(t^{1/2}\). In the case that the aquifer is uniform, the self-similar interface shape and extent is controlled by the viscosity ratio between the two fluids and a parameter that measures the importance of buoyancy-driven slumping relative to the pressure owing to fluid injection in driving the flow. In the case that injection dominates, the PDE admits shock-type solutions if the injected fluid is more viscous than the ambient and rarefaction-type solutions if the injected fluid is less viscous. We show that heterogeneity significantly alters these solutions and can even lead to suppression of the rarefaction-type solutions, for a less viscous injectate, into shocks. Contrarily, in the buoyancy-dominated regime, the influence of permeability variations is negligible. The injected buoyant fluid spreads beneath the top boundary and its evolution is controlled by the permeability in this region. The flow structure is identical to that in a uniform aquifer. Finally, we discuss the implications of these results in the context of CO2 sequestration, demonstrating that the different regimes and corresponding interface structures have a major impact on the proportion of an aquifer that can be invaded by CO2.

11:50am - 12:10pm

**An asymptotic approach to flow in pipes of triangular cross section**

**Laura Marie Keane\(^1\), Iain R. Moyles\(^1,2\), Cameron L. Hall\(^1,3\)**

\(^1\)MACSI, Department of Mathematics and Statistics, University of Limerick, Limerick, Ireland; \(^2\)Department of Mathematics and Statistics, York University, Toronto, Canada; \(^3\)Department of Engineering Mathematics, University of Bristol, Bristol, UK

The study of flow though porous media has applications in many different areas, including oil recovery processes, hydrology, and blood perfusion. These applications often require an understanding of the macroscopic flow profile in a realistic pore geometry. However, quite often the flow problem involves multi-phase fluids with interfaces of non-zero contact angle and therefore a triangular pore geometry is often used. This creates complex problems at both the pore and macroscales. Often, one way of subverting the dual complexity is to make a geometric approximation of the pore-scale flow and upscale to a network model of the pore geometry. This makes the macroscopic flow model dependent on the pore scale geometric assumptions used leading to different results for different approximations with little consideration to accuracy.

In this talk we explore single phase flow in pores with triangular cross sections at the pore-scale level. We use analytic and asymptotic methods to calculate the flow profiles of near-equilateral triangles. We show that the analytical solution agrees favourably with numerical simulations and compare and contrast our results to some of the geometric approximations used in literature. We explain how our model could be incorporated into a network model of macroscopic flow.
### Dispersion in Periodic Networks

**Yahya Farah, Alexandra Tzella**  
University of Birmingham, United Kingdom

The dispersion of a passive scalar released suddenly inside a fluid flowing through a periodic network is often described as a Gaussian approximation parameterised by an effective diffusivity. This description is, however, only valid at distances $O(t^{1/2})$ away from the centre of mass, where $t$ is the time from the scalar release. An alternative description is based on a large-deviation rate function which is valid at much larger distances $O(t)$ away from the centre of mass. In this talk, we generalise the latter approximation to describe how scalar dispersion is affected by changes in the underlying network geometry.

### The effect of compression on filtration performance

**Jakub Kory, Ian Griffiths, Armin Krupp, Colin Please**  
University of Oxford, United Kingdom

Deformations arising from an applied pressure difference in filtration impact on a filter's permeability. How should we choose the initial permeability of a filter so that it performs at its best during operation? We study the effects of filter compression using a one-dimensional model consisting of Darcy's law (modelling fluid flow) and the Navier equation (modelling the poroelastic medium). We explore filtration performance and determine the required rest-state permeability that maximises flux during operation.

### Shallow-water sloshing with wetting/drying

**Matthew Turner, Thomas Bridges**  
University of Surrey, United Kingdom

In this talk we consider the sloshing motion of two inviscid, incompressible, immiscible, shallow-water fluid layers in a rectangular vessel with a rigid lid. The vessel is forced to oscillate in a horizontal rectilinear motion, at the lowest resonant frequency of the system, such that the lower fluid hits the rigid lid causing a wetting-drying scenario. The shallow-water equations are solved with a semi-Lagrangian time-stepping procedure and results comparing the results of the scheme to experiments are presented.

### To break or not to break: The influence of invariant solutions on the transient behaviour of an air bubble in a perturbed Hele-Shaw cell.

**Jack Samuel Keeler, Gregoire Lemoult, Alice Thompson, Andrew Hazel, Anne Juel**  
University of Manchester, United Kingdom

We consider the propagation of a finite air bubble through a viscous fluid-filled Hele-Shaw channel of non-rectangular cross-section. Recent experimental work at the Manchester Centre for Nonlinear Dynamics (MCND) has revealed that the transient dynamics of a single bubble becomes increasingly complicated as the extraction rate of the fluid is increased; characterised by the formation of an increasing number of bubble tips. Depending on the size of the bubble, the bubble may eventually break-up into two or more bubbles or exhibit an oscillatory mode of propagation. To understand these dynamics we model the system using a 2D depth-averaged set of equations, and solve these equations using a finite element discretisation to reveal a rich bifurcation structure. For intermediate flow rates, there is a finite region of bi-stability: a stable asymmetric bubble solution is always present; a second solution propagates at lower speeds and transitions between a symmetric and asymmetric bubble. Two Hopf bifurcations exist on this second branch that indicate the presence of limit cycles. To quantify these limit cycles, we perform a numerical weakly nonlinear stability analysis (that can be readily applied to other systems) which provides a semi-analytic approximation to the location, size and stability of the invariant fixed points and limit cycles. Fully nonlinear simulations are consistent with this analysis and evidence is presented that the unstable periodic orbits are edge states of the system, states which mark the `boundary' between stable behaviour and the bubble breaking up. Finally these theoretical results are compared to recent experiments at the MCND.

### Levitation by Thin Viscous Layers

**Tom Mullin**  
University of Oxford, United Kingdom

The results of experimental investigations into balancing a block on a vertical moving wall which is covered with a thin layer of viscous fluid are discussed. It is found that balance can be achieved over a narrow range of speeds. Good accord is found with predictions of a lubrication model. In most cases, an essential feature of the flow is the creation of a thin tongue of viscous fluid which propagates down the wall.

*Joint work with Hilary & John Ockendon and Peter Howell

The work of TM is supported by a Leverhulme Emeritus Fellowship
Towards a model of an inflatable aerofoil: the dynamics of an elastic cell in a uniform stream

Adam Alexander Yorkston
University of East Anglia, United Kingdom

The use of inflatable wings for unmanned aerial vehicles is appealing because of their low cost, light weight and portability, and also because of their tendency to survive minor collisions better than a rigid wing. We present a study of the behaviour of a two-dimensional elastic cell in an inviscid fluid flow that works towards an understanding of the dynamics of an inflatable aerofoil. We begin very simply by studying the dynamics of a weightless elastic cell with a circular rest state that is carried in a uniform stream. Using a conformal mapping method we demonstrate a rich solution space of steady cell shapes, including cells with a left-right asymmetry and cells with a top-bottom asymmetry. We study the linear stability and subsequent nonlinear dynamics of the cell first assuming a constant pressure interior and then allowing for motion in the interior. In the last part of the talk we will cater for heavy cells by introducing circulation to effect an upwards lift force, and move toward a more realistic aerofoil-type shape by including a fixed-angle corner at the trailing edge.

11:30am - 1:00pm
Contributed Talks 9: Droplets 1
Session Chair: Carlos Antonio Galeano Rios

11:30am - 11:50am
Bouncing off the Walls: Gas-Kinetic & van der Waals Effects in Drop Impact

James Edward Sprittles1, Duncan Lockerby2, Mykyta Chubynsky1, Kirill Belousov2
1University of Warwick, United Kingdom; 2ITMO, St Petersburg

A model is developed for liquid drop impact on a solid surface that captures the thin film gas flow beneath the drop, even when the film's thickness is below the mean free path in the gas so that gas kinetic effects (GKE) dominate. Simulation results agree with experiments, with the impact speed threshold between bouncing and wetting reproduced to within 5%, while a model without GKE overpredicts this value by at least 50%. To isolate GKE, the pressure dependence of the threshold is mapped and provides experimentally verifiable predictions. There are two principal modes of contact leading to wetting and both are driven by a van der Waals driven instability of the film.

11:50am - 12:10pm
Quasi-normal free-surface impacts, capillary walking and an application to droplets.

Carlos Antonio Galeano Rios1, Paul Antoine Milewski1, Jean-Marc Vanden-Broeck2
1University of Bath, United Kingdom; 2University College London, United Kingdom

We introduce a model for successive bounces of capillary-scale objects on the free surface of an incompressible fluid bath as they translate (“walk”) along the surface. The impactors are assumed to be rigid spheres, and we consider the case for which walking velocities are small with respect to the vertical component of the impact speed. We show that the resultant problem can be decomposed into an axisymmetric vertical impact and non-axisymmetric unforced surface waves. The method imposes only the natural kinematic and geometric constraints and yields detailed predictions of the changes in the contact area and pressure field during each impact. We then apply this to simulate droplets walking on a vertically oscillating bath and compare the results to experimental reports available in the literature with remarkable agreement. We show that this model is able to capture the recently discovered phenomena of “superwalking” droplets.

12:10pm - 12:30pm
Droplet impact onto complex substrates: pre-impact dynamics

Gavin Moreton
University of East Anglia, United Kingdom

We model a droplet of water which is falling towards a solid substrate. We pay particular attention to the time close to touchdown when the droplet is becoming deformed by the reaction of the cushioning air layer. The deformation is caused by rising pressures in the layer of air between the droplet and the solid substrate. This deformation can lead to a trapped bubble of air. Two examples where such impact processes are important are in ice formation on aircraft wings, and in ink jet printing.

Oblique impacts with solid walls and the inclusion of surface tension, introduces further parameters into the model, and these have been treated by others. This talk will focus on liquid impacts with porous layers, and we present results for a variety of layer-depths and porosities.

11:30am - 1:00pm
Contributed Talks 3: Optimization and control theory
Session Chair: Vladimir Turetsky

11:30am - 11:50am
High performance computing approach to the max-cut problem

Timotej Hrga, Janez Povh
University of Ljubljana, Slovenia

Many problems in combinatorial optimization can be formulated as constrained binary quadratic problems (BQPs), which are in general NP hard. To evaluate the performance of approximation algorithms we need to solve to optimality constrained BQPs on problem instances as big as possible. In this paper we present a method for finding exact solutions of large-scale linearly constrained binary quadratic programming problems. Our exact solution method combines parallelization techniques and exact penalty method approach to obtain optimal solutions of problems of sizes that are due to their size unsolvable by existing methods and tools. We
use exact penalty method to first efficiently transform constrained BQP into an instance of max-cut, the
problem of finding a cut of maximum weight in a weighted graph. The obtained problem is then solved by
parallel branch-and-bound algorithm that uses SDP based relaxations and is implemented using MPI
(distributed memory parallel model).

11:50am - 12:10pm
Input restoration by a linear-quadratic tracking control
Vladimir Turetsky
Ort Braude College of Engineering, Israel

A problem of an input signal restoration based on the noised output measurements arises in various
applications (measurements, metrology, guidance, etc.). In the case where the system is an integrator
(cascade of integrators), the problem becomes the problem of stable signal differentiation (multiple
differentiation). This problem is ill-posed and needs a regularized solution. The proposed solution is provided
by a realization of an optimal tracking control strategy in an auxiliary linear-quadratic optimal control problem.
The tracking function is the observed system output. The regularization is achieved by including the control
integral penalty term into the cost functional. This term plays the role of the Tikhonov’s stabilizer. It is shown
that, subject to a mutual condition on the regularization parameter (penalty coefficient) and the integration
step, the numerical procedure is stable. Simulation results are presented.

12:10pm - 12:30pm
Semi-global incremental input-to-state stability of Lur’e systems.
Max Edward Gilmore, Chris Guiver, Hartmut Logemann
University of Bath, United Kingdom

Lur’e systems comprise the feedback interconnection of a linear controlled and observed system with a
nonlinearity. They are a well-studied class of nonlinear differential equations arising in numerous systems
and control theoretic contexts. The inclusion of exogenous forcing, or inputs, is very natural in applied
settings, and allows the study of the effects of disturbances generated by, for example, unmodelled dynamics,
sampling and actuation errors. It is known that forcing in nonlinear differential equations may have drastic
destabilizing effects. I shall present recent research on so-called semi-global incremental input-to-state
stability which, roughly, provides bounds on the difference of two state trajectories in terms of the differences
of corresponding initial conditions and inputs. A consequence of our stability results is a natural condition
which guarantees that the trajectories generated by (almost) periodic forcing, are asymptotically (almost)
periodic. This talk is based on joint research with Chris Guiver (Bath) and Hartmut Logemann (Bath).

12:30pm - 12:50pm
A New PDE-constrained Optimization Framework for Multiscale Particle Dynamics
Mildred Aduamoah
The Maxwell Institute Graduate School in Analysis & its Applications, United Kingdom

A vast number of important applications in mathematics and engineering are governed by mathematical
optimization problems. One crucial class of these problems that have gained significant recent attention are
PDE-constrained optimization problems, which can be used to model problems from fluid flow, industrial
processes, and biological mechanisms. However, to date, relatively little has been done by way of devising a
systematic approach to tackle multiscale PDE-constrained optimization problems arising from particle
dynamics. In this talk, we will introduce particle dynamics optimization models, discuss the real life
applications they arise from, and explain the new numerical methods that we have developed to solve them.

11:30am - 1:00pm
Contributed Talks 32: Mathematical and statistical physics
Session Chair: Vitaliy Kurlin

11:30am - 11:50am
Zero Temperature Limit of the Tight Binding Model for Point Defects
Jack Thomas, Christoph Ortner
University of Warwick, United Kingdom

In (Chen, Lu, Ortner, 2016), a tight binding model for point defects is formulated in the canonical ensemble
with finite temperature. The limiting model as domain size grows to infinity is shown to be formulated in the
grand-canonical ensemble with Fermi level fixed corresponding to the perfect crystal. In the present work, we
extend these results to the more common zero temperature models under the assumption that the Fermi level
is not an eigenvalue of the limiting Hamiltonian. In particular, we formulate zero temperature models in the
grand-canonical ensemble and prove these are consistent with taking zero temperature and thermodynamic
limits in the finite temperature models. As an application of the aforementioned results, we obtain qualitatively
sharp estimates on the interaction range for the zero temperature electronic structure model.

11:50am - 12:10pm
Discrete Coagulation-Fragmentation Systems
Lyndsay Kerr, Matthias Langer, Wilson Lamb
University of Strathclyde, United Kingdom

The coagulation-fragmentation (C-F) equations describes the evolution of clusters of particles as they break
up to produce smaller clusters and merge together to produce larger clusters. These equations have many
applications in nature and industrial processes. For example, they have been used in biological applications
to model population dynamics by, for example, Ackleh in `Parameter Estimation in a Structured Algal

When cluster size/mass is considered to be a discrete variable, the C-F equations take the form of an infinite system of ODEs. The nth equation in the system describes how the density of clusters of size n changes with time. In this talk I will concentrate on pure fragmentation. By posing the pure fragmentation system as an operator equation in a relevant sequence space, I will show how the theory of operator semigroups can be used to obtain a unique solution to the fragmentation system for suitably restricted initial conditions. Moreover, this solution can be shown to have physically relevant properties such as non-negativity and mass conservation. We are also able to draw conclusions regarding the asymptotic behaviour of solutions. In particular, under additional assumptions we can deduce that the solution of the fragmentation system decays to zero with exponential rate and we can quantify this exponential decay. In the case where mass is conserved, we can similarly show that the solution decays to the state where there are only clusters of size one present.

12:10pm - 12:30pm

From asymptotics to exact results: Painlevé I equation and 2d gravity

Ines Aniceto1, Ricardo Schiappa2, Marcel Vonk3

1University of Southampton, United Kingdom; 2IST Lisbon, Portugal; 3University of Amsterdam, Netherlands

The so-called minimal conformal field theories are often used as simple models to understand ideas of quantum gravity in physics. The simplest of these "minimal models" is 2d gravity, and the perturbative expansion of its partition function is asymptotic and formally satisfies the Painlevé I equation. This equation can be used as a toy example to study general non-linear features not only of 2d gravity but also different non-linear models.

The known asymptotic properties of the solutions of Painlevé I are connected to the existence of exponentially small contributions to the partition function of the minimal models not captured by a perturbative analysis. The theory of resurgence perfectly captures this perturbative/non-perturbative connection and its consequences. Moreover, it allows us to construct a full non-perturbative solution from perturbative data.

This talk will demonstrate the essential role of resurgence theory, coupled to exponentially accurate numerical methods, in going beyond the perturbative results and obtain (analytically and numerically) non-perturbative data. In particular it will exemplify how these techniques can be applied to the calculation of zeros of Painlevé I solutions.

12:30pm - 12:50pm

A continuous approach to a classification of solid crystalline materials

Vitaliy Kurlin

Materials Innovation Factory, University of Liverpool, United Kingdom

Solid crystalline materials (briefly, crystals) underpin key technologies such as solar cells, high-temperature superconductors and efficient photocatalysts to extract hydrogen fuel from sunshine and water. A crystal is a periodic framework based on a unit cell (a non-rectangular box) containing molecules, atoms or ions that are periodically translated in 3 directions. Functional properties of a crystal are determined by geometric positions of its atoms.

A traditional approach to predict a crystal structure based on a given chemical composition is to optimise geometric positions of atoms through slow simulations. Resulting datasets of thousands (or even millions) of hypothetical crystals contain many similar crystals often clustered around shallow local minima of an energy that indicates a thermodynamic stability of crystals.

The key obstacle in understanding which crystals are similar is an enormous ambiguity of the current representations based on a unit cell. Exactly the same crystal can be defined by infinitely many different unit cells. Though any crystal has a unique Niggli’s reduced cell, this cell is unstable under atomic perturbations. A classical approach to a classification of crystals uses discrete invariants such as symmetry groups, which are also unstable and put geometrically close crystals into different classes. Since geometric positions of atoms are continuous (not restricted to a fixed grid), crystals are more naturally classified by continuous invariants that are stable under atomic perturbations. The talk will outline a new continuous approach that rigorously quantifies a similarity between crystals by a proper metric (a distance function) based on geometric invariants.

Then different crystals (metastable polymorphs) with the same chemical compositions can be connected by continuous transition paths through lowest energy barriers. Such a continuous map on the space of all crystals will show which shallow minima should be merged with closely located deeper minima that represent realistic crystals.

The ultimate aim is to resolve the “embarrassment of over-prediction” when computer power only generates more hypothetical crystals without accurately predicting most promising materials. Parts of this work are done in collaboration with colleagues at the Materials Innovation Factory including the groups of world-leading materials scientists Prof Andrew Cooper FRS and Prof Matthew Rosseinsky FRS.
Deformations of cell sheets are ubiquitous in early animal development, often arising from a complex and poorly understood interplay of cell shape changes, division, and migration. In this talk I will describe an approach to understanding such problems based on perhaps the simplest example of cell sheet folding: the "inversion" process of the algal genus Volvox, during which spherical embryos literally turn themselves inside out through a process hypothesized to arise from cell shape changes alone. Through a combination of light sheet microscopy and elasticity theory a quantitative understanding of this process is now emerging.

**3:00pm - 3:30pm**

Coffee break

**3:30pm - 5:00pm**

Minisymposium 25B: IMA Lighthill-Thwaites Prize Presentations

Session Chair: Alan R Champneys

**3:30pm - 4:00pm**

**Optimization of mixing in stirred, binary fluids**

**Maximilian F. Eggl, Peter J. Schmid**

Imperial College London, United Kingdom

Mixing is a process that is present in a wide-range of industrial applications. Therefore, it seems imperative to optimize these processes with respect to time and energy. To this end, we present a computational framework based on nonlinear direct-adjoint looping for the optimization of mixing processes in a binary fluid system. The governing equations consist of the nonlinear Navier-Stokes equations, complemented by a time-evolution equation for the passive scalar. Immersed and moving stirrers are treated by a Brinkman-penalization technique, and the full system of equations is solved using a Fourier-based pseudospectral approach. The adjoint equations provide gradient and sensitivity information which is in turn used to enhance the efficiency of the mixing strategy, consisting of shape, rotational and path information. The geometry considered is two-dimensional in nature and consists of two cylindrical stirrers which travel on circular paths of different radii. Starting with an initial mixing strategy, the direct and adjoint governing equations are solved, after which the gradient information contained in the adjoint variables is used, together with an unconstrained optimization algorithm, to gradually progress towards a more effective strategy. The velocity along defined paths as well as the stirrer geometry will be adjusted to achieve a more homogeneous mixture over a given time horizon and within a given energy budget. Several cases of mixing enhancement, where we will vary the final time as well as optimization parameters, will be presented to demonstrate the effectiveness, efficiency and flexibility of the computational direct-adjoint approach. In all cases, significant improvements in mixing can be observed.

**4:00pm - 4:30pm**

**The Unified Transform: A New Tool for Scattering Problems**

**Matthew Colbrook**

University of Cambridge, United Kingdom

The interaction of acoustic or hydrodynamic fluctuations with thin elastic structures arise in numerous situations including both aeroacoustics, where elasticity of a wing is known to reduce the aerodynamic noise scattered by the sharp trailing edge, and oceanography, where ice sheets deform elastically on the ocean surface affecting acoustic scattering in the ocean beneath. Accurate and fast modelling of the fluid-structure interaction is key to predicting the effect of external forces on an elastic plate, or the effect of elasticity on the radiated field, and thus key for providing insight into a wide range of fluid dynamic problems. However, these types of problems are very difficult to analyse via traditional methods such as the Wiener-Hopf technique due to the complexity of the elastic kernel function (this becomes more difficult for finite structures due to the need to factorise a matrix kernel rather than a scalar kernel).

I will present a new boundary spectral collocation method for tackling such external acoustic scattering problems which may involve both rigid and elastic flat-plate boundaries. The method is ideally suited to mixed boundary value problems in unbounded domains and can handle solutions with corner singularities. The new method is fast and accurate, even for high frequencies, avoiding complications such as the evaluation of singular integrals that arise in typical boundary based methods. The method will be illustrated by application to aerodynamic noise generated by flexible wings.

**4:30pm - 5:00pm**

**Sticking with droplets: Insect-inspired modelling of capillary adhesion**

**Matthew David Butler, Finn Box, Thomas Robert, Dominic Vella**

University of Oxford, United Kingdom

Many organisms are capable of adhering to a wide variety of substrates. Insects are a particularly impressive example, having been observed to remain attached even when experiencing loads greater than 100 times bodyweight. It's generally believed that this adhesion is due to the action of the surface tension of an oily fluid that is secreted beneath their feet: the insect uses capillary adhesion. We begin by reviewing the standard model of this capillary adhesion—a droplet confined between two rigid plates—before considering how additional physical effects can improve adhesion. In particular, we will show that having a deformable foot can give rise to a significantly enhanced adhesion due to a positive feedback between capillarity and deformation. This also allows for new control and detachment strategies to be exploited.
For most frequencies, strong trapping has a weak effect in frequency-domain scattering

**David Lafontaine**, Euan Spence, Jared Wunsch

1Department of Mathematical Sciences, University of Bath; 2Department of Mathematics, Northwestern University

It is well known that when the geometry and/or coefficients allow stable trapped rays, the solution operator of the Helmholtz equation, a.k.a. the cut-off resolvent of the Laplacian, grows exponentially through a sequence of real frequencies tending to infinity.

The result we will present show that, even in the presence of the strongest-possible trapping, if a set of frequencies of arbitrarily small measure is excluded, the Helmholtz solution operator grows at most polynomially as the frequency tends to infinity.

One significance application of this result is in the convergence analysis of several numerical methods for solving the Helmholtz equation at high frequency that are based on a polynomial-growth assumption on the solution operator: our result shows that this assumption holds, even in the presence of the strongest-possible trapping, for most frequencies.

The halfspace matching method for scattering problems in infinite complex media: the dissipative case

**Sonia Fliss**, Anne-Sophie Bonnet-Ben Dhia, Patrick Joly, Yohanes Tjandrawidjaja, Antoine Tonnoir

1POEMS, ENSTA, France; 2LMI, INSA Rouen

We are interested in the scattering of time-harmonic waves in infinite complex media. The complexity of the media comes from the nature of the equations (Maxwell's or elasticity equations), its physical characteristics (periodic or anisotropic coefficients) and/or even its geometry (infinite 2D or 3D media or 3D plates). Solving time harmonic scalar waves equations in infinite homogeneous media is an old topic and there exist several methods. They are all based on the natural idea of reducing the pure numerical computations to a bounded domain containing the perturbations (achieved using for instance Finite Element methods), coupled with, for example, integral equation techniques, transparent boundary conditions involving Dirichlet-to-Neumann operators or the PML techniques. However it seems that all these methods either do not extend to complex media or do extend but with a tremendous computational cost.

By contrast, our method is based on a simple and quite general idea: the solution of halfspace problems can be expressed thanks to its trace on the edge of the half-space, via the Fourier transform in the transverse direction in the homogeneous case or via the Floquet-Bloch Transform in the periodic case.

The idea in 2D is then to split the whole domain into five parts:

- a square that includes the defect (and all the inhomogeneities) in which we will use a Finite Elements representation of the solution,
- and 4 half-spaces, parallel to the four edges of the square in which the medium is "not-perturbed", i.e. homogeneous or periodic.

We have then to couple the several integral representations of the solution in the half-spaces with a Finite Element (FE) computation of the solution in the square. By ensuring that all these representations match in the intersections, we end up with a system of equations coupling the traces of the solution on the edges of the half-spaces with the restriction of the solution in the square. In the case of a dissipative medium, the continuous formulation is proved to be coercive plus compact, and the convergence of the discretization is ensured.

In this presentation, we present the method and its analysis on a toy problem and we will explain how it extends to more complex situations.

The halfspace matching method for scattering problems in infinite complex media: the non-dissipative case

**Anne-Sophie Bonnet-Ben Dhia**, Simon Chandler-Wilde, Sonia Fliss, Christophe Hazard, Karl-Mikael Perfekt, Yohanes Tjandrawidjaja

1POEMS (CNRS-INRIA-ENSTA ParisTech); 2University of Reading

A method called Half-Space Matching (HSM) method has been developed for scattering problems in unbounded domains. The method can be used as soon as analytic representations of the scattered field are available in several half-spaces (half-planes in 2D) covering the whole domain, except a bounded region which contains the scatterer. The formulation involves second-kind integral equations coupling the traces of the scattered field on the infinite boundaries of the half-spaces. The interest of this approach is that the HSM can be used for problems which cannot be treated by classical approaches (anisotropic media, junction of open waveguides, etc...).

But up to now, even if the method works very well in practice in the non-dissipative case, the theoretical justification has been done only in the dissipative case (with a complex wavenumber).

The subject of this contribution is to present recent advances concerning the non-dissipative case. More precisely, for the case of a 2D Helmholtz equation, a complexified version of the HSM formulation has been derived, where the unknowns are now some analytic extensions of the traces of the scattered field, obtained by complex scaling. Contrary to the traces themselves, the new unknowns belong to L2 (they are even exponentially decaying at infinity).

The new formulation is proved to be of Fredholm type and well-posed. In practice, the introduction of the complex scaling in the HSM method does not require much modifications in the implementation, and the first numerical results show a better accuracy, compared to the initial formulation.
Wave-mean flow interactions in dispersive hydrodynamics: a new take on the old problem

Gennady El¹, Thibault Congy¹, Mark Hoefer²

¹Northumbria University, United Kingdom; ²University of Colorado Boulder, United States

The interaction of waves with a mean flow is a fundamental and longstanding problem in fluid mechanics. The key to the study of such an interaction is the scale separation, whereby the length and time scales of the waves are much shorter than those of the mean flow. The wave-mean flow interaction has been extensively studied for the cases when the mean flow is prescribed externally—as a stationary or time-dependent current (a “potential barrier”).

In this talk, I will describe a new type of the wave-mean flow interaction whereby a short-scale “wave projectile”—a soliton or a linear wave packet—is incident on the evolving large-scale nonlinear dispersive hydrodynamic state: a rarefaction wave or a dispersive shock wave (DSW). Modulation equations are derived for the coupling between the soliton (wavepacket) and the mean flow in the nonlinear dispersive hydrodynamic state. These equations admit particular classes of solutions that describe the transmission or trapping of the soliton (wavepacket) by an unsteady hydrodynamic state. Two adiabatic invariants of motion are identified in both cases that determine the transmission, trapping conditions and show that solitons (wavepackets) incident upon smooth expansion waves or compressive, rapidly oscillating DSWs exhibit so-called hydrodynamic reciprocity. The latter is confirmed in a laboratory fluids experiment for soliton-hydrodynamic state interactions.

The developed theory is general and can be applied to integrable and non-integrable nonlinear dispersive wave equations in various physical contexts including nonlinear optics and cold atom physics. The talk is based on the recent papers [1] - [3].

Integrability and continuous wave instabilities: an algebraic-geometric approach

Sara Lombardo

Loughborough University, United Kingdom

A direct construction of the eigenmodes of the linearization of 1+1, multicomponent, nonlinear, partial differential equations of integrable type has been introduced. This construction employs only the associated Lax pair, with no reference to spectral data and boundary conditions. In particular, this technique allows to study the instabilities of continuous wave solutions in the parameter space of their amplitudes and wave numbers, as well as to compute and potentially classify the so-called stability spectra. In the context of modulation instability, it provides also a necessary condition in the parameters for the onset of rational solitons.

The theory will be presented using the example of a system of two coupled nonlinear Schrödinger equations in the defocusing, focusing and mixed regimes. The derivation of the stability spectra is completely algorithmic and make use of elementary algebraic-geometry. It turns out indeed that, for a Lax Pair that is polynomial in the spectral parameter, the problem of classifying the spectra is transformed into a problem of classification of certain algebraic varieties. The method is general enough to be applicable to a large class of integrable systems.

If time will allow, different applications of this theory will be illustrated, including the resonant interaction of three waves.

This work has been carried out in collaboration with Antonio Degasperis (Roma “La Sapienza”) and Matteo Sommacal (Northumbria University).

Nonlinear waves in layered elastic waveguides and zero-mass contradiction

Karima R. Khusnutdinova, Matthew R. Tranter

Loughborough University, United Kingdom

In this talk I will discuss construction of a weakly-nonlinear solution of the Cauchy problem for the Boussinesq-Klein-Gordon (BKG) equation in the class of periodic functions on an interval of finite length. The equation, and the need to address this issue, have emerged in the studies of longitudinal bulk strain waves in elastic waveguides with imperfect interface. We develop a multiple-scales procedure for the derivation from the oscillating mean value, working with the equation with variable coefficients. The procedure involves fast characteristic variables and two slow time scales and averaging with respect to spatial variable, which allows us to construct an explicit and compact d’Alembert-type solution of the nonlinear problem in terms of solutions of two Ostrovsky equations emerging at the leading order and describing the right- and left-propagating waves. Validity of the constructed solution is illustrated numerically for a number of instructive examples. Importantly, in all cases the initial conditions for the leading-order Ostrovsky equations by construction have zero mass, while initial conditions for the BKG equation can be arbitrary. Thus, the so-called zero-mass contradiction has been by-passed.
Designing networks with specified spectra

Aden Forrow¹, Francis G. Woodhouse¹, Jorn Dunkel²
¹University of Oxford, United Kingdom; ²Massachusetts Institute of Technology

Complex real-world phenomena across a wide range of scales, from aviation and internet traffic to signal propagation in electronic and gene regulatory circuits, can be efficiently described through dynamic network models. In many such systems, the spectrum of the underlying graph Laplacian plays a key role in controlling the matter or information flow. To complement the traditional procedure of constructing graph ensembles with predefined statistical adjacency characteristics, I will present a mathematically rigorous weighted graph construction that exactly realizes any desired spectrum. I will then illustrate the broad applicability of this approach by showing how gapped spectra can be used to control the dynamics of various archetypal physical systems, such as controlling pattern formation in a generic Swift-Hohenberg model. The construction can be generalized to design continuous band gaps through periodic extensions of finite networks and also used to optimize spectra of networks with constrained topology.

4:00pm - 4:30pm

Modelling structural determinants of ventilation heterogeneity: a perturbative approach.

Carl A Whitfield, Alex Horsley, Oliver E. Jensen
University of Manchester, United Kingdom

We present a computational model of gas mixing and ventilation in the human lung represented as a bifurcating network. We use this to simulate lung function tests (multiple breath washout) with airway constrictions applied inter-regionally to imitate disease mechanisms. We found that impaired lung function was only detected for a range of severe constrictions that reduce airway radius to between 10%-30% of healthy values. These results help to explain the success of this particular lung function test to distinguish obstructive lung conditions from healthy controls.

We extend this model to account for intra-regional airway heterogeneity using a perturbative approach that avoids modelling each airway individually. We show also how this can be used with patient-specific airway models as well as the idealised model presented here. This method is a computationally efficient way to probe the lung’s sensitivity to structural changes, and to quantify uncertainty in predictions due to random variations in lung mechanical and structural properties.

4:30pm - 5:00pm

Network models for melt ponds on sea ice

Michael John Coughlan, Sam Howison, Ian Hewitt, Andrew Wells
University of Oxford, United Kingdom

Arctic sea ice forms a thin layer at the ocean surface, mediating key climate feedbacks. During summer, surface melting produces considerable volumes of water, which collect on the ice surface in ponds. These ponds have long been suggested as a contributing factor to the discrepancy between observed and predicted ice extent. Much work has been done to understand ponds in recent years and some attention has been paid to connected systems of ponds, which have a complicated fractal geometry and vary in area from tens of square meters. Increases in pond depth and area leads to further increases in overall melting of ice floes, contributing to the ice-albedo feedback.

Previous modelling work has focussed either on the physics of individual ponds or on the statistical behaviour of systems of ponds without much attention to physics. I will present a physically based network model for systems of ponds, which can examine both the individual and collective behaviour of ponds. Each pond initially occupies a distinct catchment basin and evolves according to an ODE representing the melting dynamics for bare and water-covered ice, and conservation of mass. Ponds can connect together to form systems in a network through fluxes of water between catchment areas, constrained by the ice topography and pond water levels.

I use the model to explore how the evolution of pond area and hence melting depends on various parameters and to explore how the connections between ponds develop over the melt season. Comparisons with observations will be made and I will discuss how the properties of the network model can inform us about real pond systems.

3:30pm - 5:00pm

Minisymposium 4A: Optimal Transport in the Analysis of Signals and Images

Session Chair: Bernhard Schmitzer
Session Chair: Matthew Thorpe

3:30pm - 4:00pm

Clustering of Big Data: consistency of a nonlocal Ginzburg-Landau type model

Riccardo Cristoferi¹, Matthew Thorpe²
¹Heriot-Watt University; ²Cambridge University

The analysis of Big Data is one of the most important challenges of the modern era. A first step in order to extract some information from a set of data is to partition it according to some notion of similarity. When only geometric features are used to define such a notion of similarity and no a priori knowledge of the data is available, we refer to it as the clustering problem. Typically this labeling task is fulfilled via a minimization procedure. Of capital importance for evaluating a clustering method is whether it is consistent or not; namely it is desirable that the minimization procedure approaches some limit minimization method when the number of elements of the data set goes to infinity. In this talk the consistency of a nonlocal anisotropic Ginzburg-Landau type functional for clustering is presented. In particular, it is proved that the discrete model converges, in the sense of Gamma-convergence, to a weighted anisotropic perimeter. The talk is based on a work in collaboration with Matthew Thorpe (Cambridge University).
4:00pm - 4:30pm

**Semi-discrete optimal transport and applications**

David Bourne  
Heriot-Watt University, United Kingdom

In this talk I will discuss an important area of optimal transport theory called semi-discrete optimal transport and its applications in image processing, economics and materials science.

4:30pm - 5:00pm

**Inverse optimal transport**

Andrew Stuart¹, Marie-Therese Wolfram²  
¹Caltech, USA; ²University of Warwick, United Kingdom

Discrete optimal transportation problems arise in various context in engineering, the sciences and social sciences. Often the underlying cost criterion is not or only partly known and the observed optimal solutions are corrupted by noise. In this talk we propose a systematic approach to infer unknown costs from noisy observations of optimal transportation plans. We illustrate the developed methodologies using the example of international migration flows. Reported migration flow data captures the number of individuals moving from one country to another in a given period of time and can be interpreted as a noisy optimal transportation map with costs related to the geographical position of countries. We use the Bayesian framework to quantify uncertainty in these transportation maps and provide estimates for moving costs.

3:30pm - 5:00pm

**Contributed Talks 5: Dynamical systems**

Session Chair: Matthew Ray Turner

3:30pm - 3:50pm

**Localized radial spots on the free surface of a ferrofluid.**

Dan J. Hill, David J. B. Lloyd, Matt Turner  
University of Surrey, United Kingdom

In 2005, Richter & Barashenkov (PRL 94.184503, 2005) published experimental evidence for the existence of axisymmetric (radial) spots on the surface of a ferromagnetic fluid, in the so-called Rosensweig instability experiment. This experiment involves a horizontal plate of ferrofluid placed between two Helmholtz coils that produce a uniform vertical magnetic field. The spots were created by placing another smaller electromagnet underneath the plate, locally increasing the applied field strength in the hysteretic region. Notably, these spots persist even after the second electromagnet is removed.

It remains a mystery as to if the existence of these spots is related to an underlying mechanism where they can spontaneously emerge from the flat state. In this talk, we provide an explanation as to why we believe the spots do emerge from the flat state and sketch out a proof, using radial centre-manifold reduction theory of Scheel (2003), for their existence close to the critical applied magnetic field strength.

3:50pm - 4:10pm

**Bifurcation of localized structures in biologically inspired reaction-diffusion equations**

Fahad Saif Al Saadi, Alan Champneys  
University of Bristol, United Kingdom

Localized structures in a Schnakenberg–like reaction diffusion models are investigated numerically and analytically. Such systems have been proposed as models for sub-cellular pattern formation and cell polarity formation through interaction between active and inactive proteins. Focussing on models in one space dimension, we use analytical techniques such as linear stability analysis, normal forms and semi-strong interaction asymptotic analysis to show the existence of two different kinds of localized structures, namely isolated spikes and localised patterns. The same state diagram is found to occur in a range of models. The results are backed up by numerical continuation of the localised states, and time simulation to check for stability. We end by studying a more realistic biological to investigate the emergence of localized structures in cell polarity due to interactions of two different families of active and inactive proteins. We find yet more complex structures, which are influenced strongly by which reaction has the stronger kinetics.

4:10pm - 4:30pm

**The 3D Painlevé Paradox**

Noah David Cheesman, John Hogan  
University of Bristol, United Kingdom

Every mathematician knows all too well that chalk can judder and squeal when pushed along a chalkboard. This phenomenon is linked to the Painlevé paradox, where no unique forward solutions exist to certain rigid body problems with unilateral constraints in the presence of friction. The Painlevé paradox has been a curiosity of mathematicians and engineers alike for over a century. But recently due to advances in mathematical techniques and the growth of the field of robotics where the problem may be especially important, there has been a surge in the study of the Painlevé paradox, both experimentally and theoretically.

In this contribution, we consider a stiff and slender rod, slipping along a rough surface. Results from developments in the 2D problem are generalised to the full 3D system. We show analytically how the planar case is singular, that the introduction of the other spatial dimension complicates the dynamics and that, whilst
in 2D no trajectories can enter the inconsistent region, in the 3D system, trajectories can enter the inconsistent region in finite time.

In order to “resolve” this paradox, one approach is regularize (smooth) the system. The method here, is to relax the rigidity of the system through adding compliance. This allows small excursions of the rod into the surface and restores determinacy. Due to the high stiffness involved, we introduce a small parameter (the compliance), leading to a slow-fast system.

4:30pm - 4:50pm

Exploring the role of directionality in shaping transition dynamics in the brain using basin stability.

Amelia J G Padmore, Martin R Nelson, Jonathan J Crofts
Nottingham Trent University, United Kingdom

Understanding structure-function relationships in the brain remains an important challenge in neuroscience. However, whilst structural brain networks are intrinsically directed, due to the prevalence of chemical synapses in the cortex, most studies in network neuroscience represent the brain as an undirected network. Here, we explore the role that directionality plays in shaping transition dynamics of functional brain states. Using a system of Hopfield neural elements with heterogeneous structural connectivity given by the Macaque cortical network, we investigate the effect of removing directionality of connections on brain capacity, which we quantify via its ability to store attractor states. In addition to determining large numbers of fixed-point attractor sets, we deploy the recently developed basin stability technique in order to assess the global stability of such brain states as well as their robustness to non-small perturbations. By comparison with standard network models with the same coarse statistics, we find that directionality effects not only the number of fixed point attractors but also the likelihood that neural systems remain in their most ‘desirable’ states. These findings suggest that directionality plays an important role in shaping transition routes between different brain networks.

3:30pm - 5:00pm

Contributed Talks 15: Physiology 2
Session Chair: Alberto Gambaruto

3:30pm - 3:50pm

Propagation of waves and transmission-reflection in stented arteries

Sara Facentese	extsuperscript{1}, Theodosios K. Papathanasiou	extsuperscript{2}, Alexander B. Movchan	extsuperscript{1}, Natasha V. Movchan	extsuperscript{1}

	extsuperscript{1}University of Liverpool, United Kingdom; 	extsuperscript{2}Brunel University London, United Kingdom

Stents are expandable tube-like devices inserted in blood vessels either to treat stenosis or aneurysms. Modelling of the dynamic response of stents is important to understand how they affect the artery-blood system.

The aim of this talk is to discuss two modelling approaches for the analysis of wave propagation in a stented artery. These include the Bloch-Floquet analysis for periodic structures and the transmission-reflection problem.

Different stent configurations are considered, e.g. overlapping stents and/or stents positioned in the same artery but separated by a gap. The analytical model is accompanied by 3D simulations.

The talk is based on the results of the recent paper [1].

3:50pm - 4:10pm

The potential of director theory to the application of cardiovascular modelling

Mikaela Joanne Webster, Alberto M Gambaruto, Alan Richard Champneys
University of Bristol, United Kingdom

The aim of this project is to investigate whether a director theory approach to modelling fluid flow in pipes could prove useful to the modelling of blood flow in the human cardiovascular system and ultimately be used as a diagnostic tool. The motive is to find an acceptable balance between accuracy and computational efficiency. The director theory approach allows for curvature of pipes and hence can provide a more realistic model of the complicated geometries of blood vessels than can classical 1D models. Yet it is simpler and hence computationally cheaper than full 3D simulations.

The idea of director theory is that the velocity of the fluid flow can be approximated by a series of director velocities which depend on the direction along the centreline of the pipe and time, multiplied by shape functions which depend on the cross-sectional coordinates. The shape functions are often chosen to be polynomials and their exact form is determined by boundary and other conditions such as continuity. Then the director velocities are solved for by taking integrated versions of the Navier-Stokes equations over the cross-section.

So far we have applied this theory to modelling fluid flow in straight and toroidally curved pipes. In straight pipes, we were able to recover the Poiseuille solution as well as a decaying swirling solution. In the toroidally curved case, the flow field matches well with a simulation run in STAR-CCM+.

4:10pm - 4:30pm

A Mathematical Model of the Pulmonary Circulation with Respiration

Jay Aodh Mackenzie, Nick A. Hill
University of Glasgow, United Kingdom
We present an analytic and computational model for blood flow and pressure in the pulmonary circulatory system that includes external pressure changes due to respiration. Such models are useful as they can aid our understanding of disease mechanisms, such as pulmonary hypertension and microvascular disease. The 1D model equations for flow and pressure in large vessels are derived from rational approximations to the Navier–Stokes equations. We use a physiologically realistic, two-sided, large vessel geometry of arteries and veins that allows pulse waves to propagate into the venous side. The sides are matched using an admittance-based boundary condition derived using a structured tree model. A structured tree is an average description of a vascular bed in which all parameters are measurable. The resulting system of equations is solved using a two-step Lax–Wendroff scheme. Flow in the main pulmonary artery is used as the upstream boundary condition and left-atrial pressure as the downstream condition.

Our model includes external pressure changes due to respiration. During inspiration the chest expands outwards and upwards, exerting negative pressure upon the lungs, pulling them open. During expiration, the chest relaxes back to its pre-inhalation state; the lungs decrease in volume. The pulmonary vasculature is also subject to this external pressure change. External (pleural cavity) pressure is measured and available in the literature.

We present simulation results that illustrate the impact of respiration on healthy pulmonary haemodynamics, and that in disease states such microvascular loss or stiffening, and pulmonary hypertension.

4:30pm - 4:50pm

Mathematical modelling of electro-mechano-fluidic coupling in the left ventricle

Hao Gao1, Kenneth Mangion2, Radostin Simitev1, Colin Berry1, Xiaoyu Luo1

1School of Mathematics and Statistics, University of Glasgow; 2British Heart Foundation Glasgow Cardiovascular Research, Institute of Cardiovascular and Medical Sciences, University of Glasgow

Cardiac disease remains one of the leading causes of death worldwide. Continuous efforts have been made towards a more complete cardiac function modelling, such as including the interactions between blood flow, myocardial mechanics and electrophysiology. Mathematical modelling of heart function is intrinsically multi-scale/physics systems of ODEs and nonlinear partial differential equations for electrical propagation and dynamics in organ level. In this work, we present a multi-physics electro-mechano-fluidic model of left ventricle (LV) developed within an immersed boundary framework with finite element elasticity.

LV geometry is reconstructed from a cardiac magnetic resonance imaging scan obtained from a healthy volunteer. Overlapped grids of different resolutions are used with a much finer grid for the electrophysiology and a coarser grid for the LV mechanics. The spread of the electrical activation and repolarization in the cardiac muscle is described by the mono-domain equation, the Ten Tusscher & Panfilov model of the human myocyte is used to describe ionic dynamics in individual myocytes. We employ the standard Galerkin finite element method for the spatial discretization of the mono-domain equation. The electrical and mechanical models are weakly coupled, that is, the solution of the mono-domain model is calculated on a static mesh, then the myocyte activation sequence is transferred to the integration points of the mechanical mesh for computing the active stress, which is described using the Niederer-Hunter-Smith’s myofilament model. The myocardium and blood interactions are described using a hybrid immersed boundary method with finite element elasticity, and finally, the systemic circulation is approximated by a three-element Windkessel model. The coupled electro-mechano-fluidic LV model is implemented in open-source packages (IBAMR and LibMesh) and solved in parallel.

The predicted LV dynamics are consistent with the observed measurements. The whole LV is activated within 69 milliseconds starting from the mid-apical endocardial surface towards epicardium and the base. The isovolumetric contraction duration lasts for 76 ms with an ejection fraction of 53.3% and a maximum aortic flow rate of 400 mL/s. In summary, the coupled multi-physics electro-mechano-fluidic model has the potential to describe the whole LV functionality and to deepen our understanding of heart diseases.

Acknowledgement: UK EPSRC EP/N014642/1, BHF PG/11/2/28474; FS/15/54/31639; PG/14/64/31043; RE-18-6134217

3:30pm - 5:00pm

Contributed Talks 27: Industrial modelling 2
Session Chair: Ferran Brosa Planell

3:30pm - 3:50pm

Homogenisation of a shrinking core model for gas-solid reactions in granular particles

Benjamin Matthew Sloman1,2, Colin Peter Please3, Robert Ashton Van Gorder3,2

1Elkem ASA; 2University of Oxford; 3University of Otago

Reactions between gases and solid particles are commonly modelled using a shrinking core framework, where a sharp interface between an inner unreacted core and an outer product shell moves inwards until the reaction is complete. However, for some physical systems, such a sharp divide is not present, and so a more accurate model is needed to capture the transition region for the reaction. We are interested in large particles made of many small grains, where there are strong interactions between microscale granular and macroscale particulate effects, and where a shrinking core model represents behaviour at the microscale level.

In this talk, we present an effective macroscale model for such gas-solid reactions, which is derived via homogenisation theory by exploiting the small ratio of granular to particle length-scales. These macroscale equations allow for a diffuse reaction front, as well as a sharp interface between reacted and unreacted solid material. We analyse the resulting model asymptotically in the limits where the reaction time is rate-limited by both chemical kinetics and diffusion, commenting on the width of the reaction zone. Numerical simulations support the law of additive reaction times, which states that the total reaction time is the sum of the conversion times under these limits. We further discuss how our results can be extended to incorporate the transport of the product gas out of the solid particle, using a binary Fickian diffusion model. In metallurgical production,
the particle size and porosity of reactants are known to influence reaction times. Our results help quantify these effects, and hence may aid in raw material selection for such processes.

3:50pm - 4:10pm

Asymptotic Analysis of Small Aspect Ratio Lithium-Ion Batteries
Robert Timms, S. Jon Chapman, Colin P. Please
University of Oxford, United Kingdom

Lithium-ion batteries are one of the most widely used technologies for energy storage, with applications ranging from portable electronics to electric vehicles. Due to their popularity, there is a continued interest in the development of mathematical models of lithium-ion batteries. Such models often assume that the battery operates in a uniform manner, leading to a simplified one-dimensional description. However, larger sized batteries, such as those used in the electric vehicle sector, exhibit non-uniform behaviour in the current and temperature distribution which can adversely affect battery performance and lifetime.

We present a three-dimensional electrochemical-thermal model describing the behaviour of a typical lithium-ion pouch cell. By exploiting the thinness of the pouch cell geometry we show that the model decouples into a one-dimensional electrochemical model in the cross-cell direction, and a simplified two-dimensional model in the perpendicular plane. We identify key parameter groupings and asymptotic limits in which the model simplifies further, allowing for efficient evaluation of the impact cell design has on battery operation.

4:10pm - 4:30pm

Asymptotic reduction of a thermal-electrochemical model for lithium-ion batteries
Ferran Brosa Planella, W. Dhammika Widanage
University of Warwick, United Kingdom

Understanding the thermal-electrochemical behaviour of lithium-ion batteries is crucial to design a new generation of batteries, as the thermal effects have a fundamental role in the ageing and degradation of the battery. The Newman model is widely used to describe the electrochemical behaviour of lithium-ion batteries, as it provides accurate predictions for a broad range of operating conditions. Furthermore, this model can easily be coupled to a thermal model to describe the evolution of temperature. However, the Newman model is computationally expensive to solve and therefore, for optimisation and control applications, reduced models become necessary. We present an asymptotic reduction of the coupled thermal-electrochemical model that can be used to obtain fast predictions of the battery temperature. We take the limit of fast transport of lithium ions in the electrolyte and large potential drop across the cell, obtaining much simpler governing equations. The transport of lithium ions in the electrode must be considered carefully as it has an important role in the relaxation mechanism that is observed during resting periods. Finally, we compare the reduced model with experimental data for commercial lithium-ion batteries.

4:30pm - 5:00pm

Thermodynamics vs molecular dynamics based models of electrochemical transport
Maxim Zyskin
University of Oxford

I will talk about thermodynamics vs molecular dynamics based multi-species models of electrochemical transport in fluids, and in particular on computing multi-species continuum transport model parameters from fluctuations regression hypothesis and molecular dynamics simulations. This has applications to modeling electric batteries, in particular.

3:30pm - 5:00pm

Contributed Talks 30: Transition to turbulence 1
Session Chair: Ashley Willis

3:30pm - 3:50pm

Buoyancy-suppressed transition in vertical pipe flow
Ashley Willis, Elena Marensi
The University of Sheffield, United Kingdom

Turbulence in the flow of fluid through a pipe can be suppressed by buoyancy forces. As the suppression of turbulence leads to severe heat transfer deterioration, this is an important and undesirable effect in both heating and cooling applications. He et al. (2016) investigated this effect via a simplified model for the buoyancy force, and attributed the suppression to a reduction in the apparent Reynolds number of the flow, as measured by the pressure gradient required to drive the flow. Meanwhile, in ordinary (isothermal) pipe flow, Kuhnen et al. (2018) observed relaminarisation attributed to flattening of the base flow profile. The flattening was introduced by a range of internal and boundary flow manipulations. Enhanced stability of a flattened base flow has been verified theoretically by Marensi et al. (2019) through its affect on the minimal seed (the smallest disturbance to a laminar flow) that triggers turbulence.

We present results of simulations and examine how travelling wave solutions, which have been shown to mediate transition to turbulence in isothermal flows (Schneider et al. 2007), are affected by axial buoyancy.

3:50pm - 4:10pm

Fractal neutral curves in stably-stratified shear flows
Jonathan James Healey
Keele University, United Kingdom
The author has recently shown that stably-stratified plane Couette flow, where the flow is a uniform shear between horizontal plates, and the fluid density increases monotonically in the downward vertical direction, has neutral curves with fractal properties for a certain family of density profiles. While plane Couette flow is linearly stable, it was known that (statistically) stable density profiles could destabilize this flow. It is surprising, however, to find fractal behaviour generated by a 2nd order linear ODE (the Taylor-Goldstein equation, widely used in geophysical fluid dynamics), as fractals are more usually associated with nonlinearity. In this conference presentation we show that this not simply a mathematical curiosity of a particular, perhaps rather artificial, flow, but can occur in arbitrary shear flows whose density profiles have a few simple properties.

4:10pm - 4:30pm

Optimal forcing to destabilise turbulence in a pipe flow
Elena Marensi¹, Ashley P. Willis², Rich R Kerswell³
¹School of Mathematics and Statistics, University of Sheffield, UK; ²Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK

Recent experiments (Kühnen et al., 2018) in pipe flow have shown that flattening the turbulent streamwise velocity profile destabilises the turbulence so that the flow relaminarises. The flattening of the mean profile was obtained in the experiments by inserting a baffle in the core of the pipe. As a first step towards capturing this phenomenon theoretically, Marensi et al. (2019) performed direct numerical simulations of pipe flows where the presence of the baffle was modelled by adding an artificial body force to the Navier-Stokes equations. With this simple form for the baffle, Marensi et al. (2019) were able to predict enhanced nonlinear stability of the laminar state and significant drag reductions, both laminar and turbulent. In an effort to push forward these encouraging first results, we construct a new fully nonlinear optimisation problem, whereby the "minimal forcing", i.e. the forcing characterised by the lowest amplitude or the minimum work done against the flow, is sought to just destabilise the turbulence. The energy input, defined as the sum of the viscous dissipation and the work done by the forcing, is significantly reduced. The resulting optimal forcing, obtained with a variety of different initial guesses and for both short and long pipes, shows a strong radial localisation close to the wall, is axisymmetric and, for sufficiently long pipes, is localised in the streamwise direction.

4:30pm - 4:50pm

Density homogenisation within stably-stratified exact coherent structures in shear flows
Jake Langham¹, Tom Eaves², Rich Kerswell³
¹University of Bristol, United Kingdom; ²Department of Mathematics, University of British Columbia; ³Centre for Mathematical Sciences, University of Cambridge

Unstable simple invariant solutions known as exact coherent structures are thought to be the building blocks of turbulent flow. We study these solutions in plane Couette flow with a stable density field added under the Boussinesq approximation. In the physical limits where density transport is dominated either by diffusion or advection, we find that states persist for high levels of global stratification, in spite of the stabilising influence of buoyancy. In the advective limit, states achieve this by homogenising in the channel interior, stratifying only in thin boundary layers at the walls. This layering, reminiscent of density layers in geophysical flows, makes the states indifferent to globally imposed density gradients. As far as we are aware, this is the first example of such layering in an invariant solution to the Boussinesq equations.

3:30pm - 5:00pm

Contributed Talks 4: Fluids 2
Session Chair: Emmanuel Dormy

3:30pm - 3:50pm

Atmospheric predictability: the origins of the finite-time behaviour
Tsz Yan Leung¹, Martin Leutbecher², Sebastian Reich³,1, Theodore G. Shepherd⁴
¹University of Reading, United Kingdom; ²European Centre for Medium-Range Weather Forecasts; ³University of Potsdam, Germany

First proposed by Edward N. Lorenz in 1969, the existence of a finite-time barrier in deterministically predicting atmospheric flows is now well-accepted in the community of dynamical meteorology. In this talk we argue via numerical simulation that Lorenz’s model may be over-simplified. The apparent contradiction between a finite-time barrier to predictability and the proof of well-posedness of the incompressible two-dimensional Navier-Stokes equations, regardless of the slope of the kinetic energy spectrum, is reconciled through understanding of this slope’s practical role in a particular error bound of the analytic proof.

3:50pm - 4:10pm

Leaky equatorial waves
Lyubov Chumakova
U. Edinburgh, United Kingdom

Understanding the dynamics of equatorial waves is essential for weather prediction and climate modelling. However, one aspect of their dynamics is often overlooked - the dissipation through vertically propagating waves. These leaky waves leave the region of interest (e.g. troposphere) and never return. Recently, we have developed a framework to study leaky waves, by extending the concept of group velocity to complex exponential waves. This was essential, since leaky waves have exponential vertical profiles and thus the standard concept of group velocity does not apply to them. This technique allows to study analytically the effect of dissipation due to radiation in more detail. In this talk I will address the effect of leakage on equatorial trapped waves.

4:10pm - 4:30pm
Mathematical modelling of heat pumps as a renewable energy source
Alistair Delboyer
University of Nottingham, United Kingdom
Investment in renewable energy systems has grown significantly over recent years to cut carbon emissions and combat climate change. One such method is to utilise heat in the environment to warm or cool buildings using low-grade heat pumps. Open water source heat pumps take water from rivers, pass it through the heat pump system, and then discharge it back into the river at a different temperature. The temperature discharge is legislated in the UK to be within 3°C of ambient. Mathematical models for the behaviour of the fluid discharged from the heat pumps are formulated in terms of buoyant plumes. The dynamics of arrays of plumes of relatively warm (or cool) water in strong cross-currents are not well understood and have ecological and efficiency implications. It is important to know how far downstream the effect of these arrays of plumes may travel before becoming negligible in order to inform where heat pumps are placed. A model is given for the behaviour of arrays of plumes in the absence of a crosswind. This can be used to calculate where there is a measurable impact on the ambient river. The model is extended to an arbitrary number of heat pumps and a model of plumes in a crosswind is also proposed.

4:30pm - 4:50pm
Eye formation in large scale vortices: mathematical models vs tropical cyclones
Emmanuel Dormy¹, Ludivine Oruba², Peter Davidson³
¹Ecole Normale Supérieure & CNRS, France; ²Sorbonne Université, France; ³University of Cambridge, U.K.
One of the most striking features of atmospheric vortices, such as tropical cyclones, is that they often develop a so-called eye: a region of reversed flow in and around the axis of the vortex. The patterns for this structure are still poorly understood. The ubiquitous appearance of eyes embedded within large-scale vortices suggests that the underlying mechanism by which they first form may be independent (partially if not wholly) of atmospheric complexities. We considered what is, perhaps, the simplest mathematical model in which eyes may form; that of steady axisymmetric Boussinesq flow. Our numerical experiments show that in this configuration, for sufficiently vigorous flows, an eye can form. I will first discuss the mechanism of eye formation and the criteria required for eye formation in the idealised model. I will then discuss the robustness of this mechanism as more « realistic » models of tropical cyclones are tackled.

3:30pm - 5:00pm
Contributed Talks 10: Droplets 2
Session Chair: Nikos Savva

3:30pm - 3:50pm
Cahn-Hilliard Navier-Stokes simulations for design of superhydrophobic surfaces
Matthew Ryan Tranter¹, Benjamin Aymard², Serafim Kalliadasis³, David N Sibley⁴
¹Loughborough University, United Kingdom; ²MathNeuro Team, Inria, France; ³Imperial College London, UK
Self-cleaning is an important feature that is desirable in many applications, such as solar panels. The effect of varying the topography of a surface can aid the ability of droplets, of rainwater for instance, to bead up, roll down, and pick up dust particles in the process. To this end we consider the motion of a two-dimensional droplet on an inclined substrate and study the effect of varying bottom topography on the motion. The model used to describe the motion is a Navier-Stokes model, incorporating gravity, coupled to a Cahn-Hilliard model for a phase-field. This model is chosen so that the droplet interface is described by an isoline of the phase-stability function. The dynamical processes for this structure are still poorly understood. The ubiquitous appearance of eyes embedded within large-scale vortices suggests that the underlying mechanism by which they first form may be independent (partially if not wholly) of atmospheric complexities. We considered what is, perhaps, the simplest mathematical model in which eyes may form; that of steady axisymmetric Boussinesq flow. Our numerical experiments show that in this configuration, for sufficiently vigorous flows, an eye can form. I will first discuss the mechanism of eye formation and the criteria required for eye formation in the model. I will then discuss the robustness of this mechanism as more « realistic » models of tropical cyclones are tackled.

3:50pm - 4:10pm
Wettability-Independent Droplet Transport by Bendotaxis
Alexander Bradley¹, Finn Box², Ian Hewitt¹, Dominic Vella³
¹University of Oxford, United Kingdom; ²University of Manchester, United Kingdom
When a drop is confined in a thin channel with deformable walls, a combination of bending and capillarity causes a pressure gradient that, in turn, results in the spontaneous movement of the liquid. Surprisingly, the direction of this motion, which we refer to as bendotaxis, is always the same, regardless of the wettability of the channel; bendotaxis may therefore be a useful means of transporting droplets on small scales, with various technological applications. This talk will present details of macroscopic experiments as well as a simple mathematical model used to study this motion, and discuss the associated time scales. The effects of geometry shall also be considered, with a particular focus on the case of interacting channels.

4:10pm - 4:30pm
The spreading and stability of a cooling drop on an inclined and prewetted substrate
Shailesh Naire, Ghanim Algwaush
School of Computing and Mathematics, Keele University, United Kingdom
Molten liquid flows that cool as they spread are important in a wide variety of contexts, e.g., lava domes in geophysical flows and coolant in nuclear reactors. The interplay between the flow and cooling can also give rise to a variety of intriguing flow features and fingering instabilities.
Motivated by the above, we consider theoretically a model system of a molten viscous drop extruding from a source and spreading over an inclined plane that is covered initially with a thin liquid precursor film. Lubrication theory is employed to model the one-dimensional spreading flow using coupled nonlinear evolution equations for the film thickness and temperature. The coupling between flow and cooling is via a constitutive relationship for the temperature-dependent viscosity. This model is parametrised by the heat transfer coefficients at both the drop-air and drop-substrate interfaces, the Péclet number, the viscosity-temperature coupling parameter and the substrate inclination angle. A systematic exploration of the parameter space reveals a variety of solutions illustrating the dynamics of a spreading fluid undergoing cooling. These solutions are compared to a simpler model that results due to a further approximation of the temperature equation in the limit of small Péclet number. The stability of the one-dimensional solutions to small-amplitude variations in the thickness and temperature in the transverse direction is also investigated. The existence of a fingering instability is revealed. A dispersion relationship is described using a transient growth analysis and numerical simulations, which elucidates the fundamental physical mechanism underlying this fingering instability.

3:30pm - 4:50pm

Droplet dynamics over heterogeneous substrates with mass transfer

Danny Groves, Nikos Savva
Cardiff University, United Kingdom

We investigate the effect of mass transfer on the dynamics of a thin, partially wetting droplet moving due to slip on a chemically heterogeneous surface. The dynamics is described by a single evolution equation for the droplet thickness arising from the long-wave expansion of the Stokes equations. By asymptotically matching the flow in the bulk to that near the contact line, we derive a simplified system of ordinary differential equations for the Fourier coefficients of the contact line in the limit of vanishingly small slip lengths, slow mass transfer rates and nearly circular contact lines. The complex features of the dynamics are uncovered by obtaining solutions for a number of representative benchmark cases. It is shown that the simplified system is able to capture the dynamics of the full system with very good accuracy and, importantly, at a fraction of the computational cost. To partially lift the restriction that the contact line must remain nearly circular, a hybrid numerical scheme based on the boundary integral method is also presented. This scheme is demonstrated to exhibit better accuracy compared to the simplified system, but at a much lower computational cost compared to the full system.

3:30pm - 3:50pm

Post-buckling analysis of soft elastic bilayers

Hamza Aderemi Alawiye
University of Oxford, United Kingdom

Wrinkling is a universal instability occurring in a wide variety of engineering and biological materials. Here, we present a combined analytical and numerical treatment of the computation of the amplitude of wrinkles in a growing, soft, hyperelastic bilayer after the occurrence of the instability. Furthermore, we consider the question of stability of the wrinkled solutions and set out a program of investigation for secondary bifurcations and other instabilities in the system.

3:50pm - 4:10pm

Biological membranes with deformations induced by point particles

Philip Justin Herbert
The University of Warwick, United Kingdom

We motivate a fourth order surface PDE which arises in the study of near spherical biological membranes, where we consider the geometry is made non-trivial by point particle inclusions. One may consider two models for study, one where the constraints are strictly obeyed, and another where the constraint is penalised (so called hard constraints and soft constraints respectively). We discuss the well posedness of these problems along with the well posedness of an appropriate splitting schemes in order to develop numerical experiments. This is joint work with Charlie Elliott.

4:10pm - 4:30pm

Multiphase and morpho-poro-elastic multiscale models of biological tissue growth

Reuben O'Dea
University Of Nottingham, United Kingdom

The derivation of so-called ‘effective descriptions’ that explicitly incorporate microscale physics into a macroscopic model has garnered much attention, with popular applications in poroelasticity, and models of the subsurface in particular. More recently, such approaches have been applied to describe the physics of biological tissue. In such applications, a key feature is that the material is active, undergoing both elastic deformation and growth in response to local biophysical/chemical cues. Here, two new macroscopic descriptions of drug/nutrient-limited tissue growth are introduced, obtained by means of two-scale asymptotics. First [1,2], a multiphase viscous fluid model is employed to describe the dynamics of a growing tissue within a porous scaffold (of the kind employed in tissue engineering applications) at the macroscopic. Secondly [3], the coupling between growth and elastic deformation is considered, employing a morpho-elastic description of a growing poroelastic medium. Importantly, in this work, the
restrictive assumptions typically made on the underlying model to permit a more straightforward multiscale analysis are relaxed, by considering finite growth and deformation at the pore scale.


4:30pm - 4:50pm
Phase field models for small deformations of biomembranes arising as Helfrich energy equilibria
Luke Hatcher
University of Warwick, United Kingdom

Small micro-domains known as ‘lipid rafts’ have been posited to form on biological membranes and are thought to play a role in many cellular processes, such as signal transduction, membrane trafficking and protein sorting. The small scales on which lipid rafts are believed to form (10-200nm) has meant their existence remains controversial. However, some support for the raft hypothesis can be found in the experimental observation of such micro-domains in artificial membranes known as giant unilamellar vesicles. It is therefore interesting to study the processes by which these rafts could be produced.

In this talk we investigate whether the geometry of the membrane could be a mechanism which drives the formation of these lipid rafts. We will derive a model for these two-phase membranes by considering the Canham-Helfrich energy with phase-dependent spontaneous curvature, and by making the simplifying assumption that the membrane remains approximately spherical in shape. We will consider the diffuse interface problem and motivate this by a formal asymptotic analysis. Finally we will discuss some numerical experiments obtained by considering a corresponding gradient flow. This is joint work with Charlie Elliott and Bjorn Stinner.

3:30pm - 5:00pm
Contributed Talks 1: Finance, economics and society
Session Chair: Cameron Luke Hall

3:30pm - 3:50pm
Preference selection of Lithuanian II pillar pension funds by stochastic dominance rules
Audrius Kabasinskas¹, Miloš Kopa², Kristina Šutienë¹
¹Kaunas University of Technology, Lithuania; ²Charles University, Czech Republic

This study contributes to the research of multi-pillar pension system, mainly focusing on the private pension funds. In this context, the specific objective of this study is to determine which private fund in the second pillar is the best for a participant on the basis of his risk profile. Depending on the assumption on the pension system participant’s utility function, the four different types of stochastic dominance (SD) relations are considered, specifically first-order, second-order, third-order and SD generated by utility functions with decreasing absolute risk aversion. We provide the analysis under three distributional assumptions: empirical, stable and truncated stable distribution of returns. Moreover, for non-dominated funds, an investor for which the fund is the optimal choice is identified. Finally, the behaviour of the participants in last quarter/year is compared to the results of SD analysis.

3:50pm - 4:10pm
Approximate filtering of intensity process for Poisson count data
Naratip Santitissadeekorn
University of Surrey, United Kingdom

We employ a Hawkes process to model the intensity rate of crime events, which is motivated by the well-known concepts of near-repeat victimization and neighborhood effects in criminology theory. In practices, however, data has to be assimilated to optimize the model in a recursive manner in order to perform a real-time prediction. We develop an approximation sequential data assimilation technique similar to the extended Kalman filter, called the extended Poisson-Kalman filter (ExPKF), where only the mean and covariance are sequentially updated using count data via the Poisson likelihood function. The ExPKF, however, is inconvenient to use when the computation of the Hessian is difficult. Thus, we also develop an ensemble-based filter based on the Gamma prior assumption; hence, ensemble Poisson-Gamma filter (EnPGF). The performances of ExPKF and EnPGF are demonstrated in several synthetic experiments where the true solution is known. For the application to real-world data, we use ExPKF to approximate the uncertainty of urban crime intensity and parameters for Hawkes process and highlight the advantage of filtering scheme (over the non-filtering scheme) to track parameter changes and how it may improve the police patrol allocation.

4:10pm - 4:30pm
Modelling the effect of externalities on auctions with multiple successful bidders
Cameron L. Hall¹, Mol T. Devine², Niall Farrell³
¹University of Bristol, United Kingdom; ²University College Dublin, Ireland; ³Potsdam Institute for Climate Impact Research, Germany

In procurement auctions (e.g. auctions to secure electricity production contracts), it can be necessary to select multiple successful bidders to meet a given deployment target. These auctions can be run in a range of different ways and the optimal bidding strategies will depend on the auction format. We have been
investigating how optimal bidding strategies are affected by factors external to the auction (externalities) that affect the relationship between the rank of a given bid and the bidder's chance of success. One model that we have used assumes that the effect of externalities can be captured with a single parameter associated with the probability that a bidder that would have been successful in the absence of externalities "misses out" and their position passes to a lower-ranked bidder. While easy to apply when one successful bidder is to be selected, this model becomes complicated when multiple successful bidders are required. In this talk, we present our model alongside a simplification that works exceptionally well when there is a large number of bidders (successful and unsuccessful). We also pose an open question on how to use asymptotic methods (or some other approach) to demonstrate the relationship between these two approaches.

Plenary 3: IMI Public Lecture
Session Chair: Christopher Budd

Applying mathematics to understand our changing climate
Emily Shuckburgh
British Antarctic Survey, United Kingdom

Global temperatures are about 1°C warmer than they were before emissions of greenhouse gases by human activities started to alter our climate. Month-after-month we see the devastating impacts of extreme weather around the world with, in many cases, the risk of occurrence increasing because of climate change. The higher the warming, the greater the risk. If warming continues at the present rate, we are likely to exceed 1.5°C sometime between about 2030 and 2050, and we are on course to exceed 3°C of warming by the end of the century.

In this talk, I will discuss how we are using mathematics – from classical dynamics to the latest developments in machine learning – to understand our changing climate and the risks posed to human society.
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<td>Sammy Petros, Daniele Avitabile, Stephen Coombes, Stamatos Sotiropoulos, Paul Houston</td>
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<td>Travelling wave solutions for a space-time fractional SIR model by the (G'/G) expansion method</td>
<td>Areej Abdullah Almuneef¹, Moustafa Elshahed², Nigel Mottram³</td>
<td>¹Department of Mathematical Sciences, Princess Nourah bint Abdulrahman University, Riyadh, Saudi Arabia; ²Unizah Faculty of Arts and Sciences, Qassim University, Saudi Arabia; ³Department of Mathematics and Statistics, University of Strathclyde, Glasgow G1 1XH, Scotland, UK</td>
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<td>Stability and instability of planar layers of smectic A liquid</td>
<td>Omar Ameer Alsuhaimi¹, Iain Stewart³, Gunnar Hornig¹</td>
<td>¹The University of Dundee, Dundee, United Kingdom, Taibah University, Saudi Arabia; ³The University</td>
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<td>Harold Heorton¹, M Tsamados¹, S Cole², A Ferreira¹, A Berbellini¹, M</td>
<td>¹UCL, United Kingdom; ²Woods Hole Oceanographic Institute USA; ³Jet Propulsion Laboratory CIT USA</td>
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<td>in-situ and satellite observations using an inverse modelling</td>
<td>Fox¹, T Armitage²</td>
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**Modelling and data analysis of epidemics**

**Julia Gog**  
University of Cambridge, United Kingdom

The study of infectious disease is one of the largest and most developed areas of mathematical biology. Yet the innate complexity of disease dynamics, the growth of many forms of available data and pressing real-world issues mean that this area is still rich with problems across a range of mathematical areas.

This talk will be focused on influenza. For seasonal influenza (the usual type of flu that circulates each winter), the challenges lie in understanding viral evolution in highly dynamic population models. For pandemics, past and recent data allows detailed exploration of the spatial dynamics, but raises many more questions. The hope is that modelling work will help mitigate the damage of future pandemics.

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**Contact line dynamics on rough and heterogeneous surfaces**

**Andreas Münch**  
University of Oxford, United Kingdom

We investigate dewetting polymer melts through their thin film models, and explore in particular their tendency to give rise to patterns. We fill focus in particular on general features, such as rim formation, retraction rates, rupture cascades and fingering phenomena, and highlight how they are affected by the conditions at the substrate, in particular slip, and compare theoretical predictions with experiments. If time permits, we will also explore the role of extensional stresses for very large slip lengths via asymptotic analysis.

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**How does imperfect adherence to antimalarials contribute to transmission? A within-host modelling approach**

**Joseph D. Challenger, Azra C. Ghani, Lucy C. Okell**  
Imperial College London, United Kingdom

Artemether-lumefantrine (AL) is the most widely recommended antimalarial worldwide for Plasmodium falciparum malaria. Clinical trials have clearly demonstrated its safety and efficacy. Effective treatment will restore the patient to health and also limit their contribution to onward transmission. Clearly treatment efficacy...
will diminish if adherence to treatment is poor, but this relationship can be hard to quantify. In previously published work, we developed a within-host model of falciparum malaria, and assessed the performance of AL, collected in Tanzania in 2012. We now develop our investigation to quantify the impact that poor adherence has on onward transmission of the parasite to an Anopheles mosquito. We extend our model to include sexual-stage parasites (gametocytes), and use clinical trial data to quantify the drug action against these parasites. We find that realistic patterns of drug adherence more than double a patient’s capacity to transmit, compared to the case where adherence is perfect. We also show how delayed access to treatment for malaria can lead to increased transmission.

11:30am - 12:00pm

A mathematical model for the community ecology of Borrelia burgdorferi strains

Ben Adams
University of Bath, United Kingdom

Borrelia burgdorferi is a complex of bacterial species found throughout Europe and North America. The epidemiological dynamics are zoonotic but some strains can cause Lyme disease in humans. Rodents and birds are important natural hosts.Ticks are responsible for transmission between vertebrates. In many regions a diverse community of Borrelia strains co-circulate. Mechanisms governing the composition of these communities are believed to include multiple niche polymorphism (MNP) and negative frequency dependence (NFD). MNP can occur when Borrelia strains are specialised to exploit particular vertebrate host species, mostly likely by evasion of innate immunity. NFD can occur when infection with one Borrelia strain elicits an adaptive immune response in the host that provides at least partial protection against re-infection with that strain and similar strains. Here we use a mathematical model to examine how Borrelia strain communities may be structured by the combined effects of host specialization and immune cross-protection, given that transmission occurs via a generalist vector.

12:00pm - 12:30pm

Correlations between stochastic endemic infection in multiple interacting subpopulations

Sophie Meakin, Matt Keeling
University of Warwick, United Kingdom

Heterogeneity is commonly incorporated into epidemiological models by dividing the population into multiple interacting subpopulations. This partitioning captures a variety of characteristics of the whole population; the subpopulations may represent: geographically separated locations, high- and low-risk groups, age structure or multiple species. The strength of interaction, or ‘coupling’, between two populations can be captured by a single phenomenological parameter; however, a limitation of this approach is how to infer this coupling parameter. Between-population interactions are complex and high quality data on relevant interactions are rarely available; how such data translates into a single coupling parameter is also unclear. We present a method that circumvents this problem by estimating the coupling using more widely-available data on disease incidence.

We begin with a stochastic SIR model in P identical interacting subpopulations, where the force of infection in each subpopulation depends on a mixture of within-population and between-population transmission. By making an analytic approximation we derive an analytic approximation for the correlation between the number of infected individuals in a given pair of subpopulations as a function of the coupling between them. We show that our result holds for a range of parameter values and is supported by stochastic simulations -- considering a measles-like disease as a specific example.

We can also reverse this process: the correlation between the number of infected individuals in two populations can be calculated from data on disease incidence and then used in conjunction with our result to estimate the coupling parameter. Crucially, this allows us to estimate the coupling between subpopulations even in the absence of data on human mobility. As heterogeneity is widely-acknowledged to promote to disease persistence, so accurate estimation of coupling parameters could be invaluable to disease eradication research.

11:00am - 12:30pm

Minisymposium 10A: Recent advances in PDE models describing emergent behaviour and collective dynamics

Session Chair: Bertram Düring
Session Chair: Marie-Therese Wolfram

11:00am - 11:30am

Derivation of macroscopic dynamics for collective motion in a fluid

Pierre Degond\(^1\), Sara Merino-Aceituno\(^2\), Fabien Vergnet\(^3\), Hui Yu\(^4\)

\(^1\)Imperial College London, UK; \(^2\)University of Vienna / University of Sussex, Austria; \(^3\)Université Paris Sud, France; \(^4\)Tsinghua University, China

We derive macroscopic dynamics for collective motion in a fluid. The starting point is a coupled Vicsek-Stokes system. The Vicsek model describes self-propelled agents interacting through alignment. It provides a phenomenological description of steric interactions (volume exclusion) between agents at high density. Stokes equations describe a low Reynolds number fluid.

11:30am - 12:00pm

Strong solutions and weak-strong stability in a system of cross-diffusion equations

Judith Berendsen
TU Chemnitz, Germany
Proving the uniqueness of solutions to multi-species cross-diffusion systems is a difficult task in the general case, and there exist very few results in this direction. In this talk, we study a particular system with zero-flux boundary conditions for which the existence of a weak solution has been proven in [Ehrlacher2017]. Under additional assumptions on the value of the cross-diffusion coefficients, we are able to show the existence of strong solutions. The proof relies on the use of an appropriate approximation and a fixed-point argument. In addition, a weak-strong stability result is obtained for this system in dimension one which implies uniqueness.

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<td><strong>Incorporating a multistage representation of the cell cycle into models of cell migration</strong></td>
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<td><strong>Kit Yates</strong></td>
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<td>University of Bath, United Kingdom</td>
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<td>The stochastic simulation algorithm commonly known as Gillespie’s algorithm (originally derived for modelling well-mixed systems of chemical reactions) is now used ubiquitously in the modelling of biological processes in which stochastic effects play an important role. However, Gillespie’s algorithm is routinely applied to model biological systems for which it was never intended. In particular, processes in which cell proliferation is important (e.g. embryonic development, cancer formation) should not be simulated naively using the Gillespie algorithm since the history-dependent nature of the cell cycle breaks the Markov process. Here we suggest a method of modelling the cell cycle that restores the memoryless property to the system and is therefore consistent with simulation via the Gillespie algorithm. By breaking the cell cycle into a number of independent exponentially distributed stages we can restore the Markov property at the same time as more accurately approximating the appropriate cell cycle time distributions. We demonstrate the importance of employing the correct cell cycle time distribution by recapitulating the results from models incorporating cellular proliferation. In particular, we analyse the effect of incorporating the multi-stage cell cycle distribution on the wave-speed in a pulled-front Fisher wave from both individual-based and continuum perspectives.</td>
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<td><strong>Minisymposium 11A: New Perspectives and Challenges at the Junction of Modelling and Applications</strong></td>
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<td><strong>Session Chair: Apala Majumdar</strong></td>
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<td><strong>On the shape of gravitating planets</strong></td>
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<td><strong>Alain Goriely</strong></td>
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<td>University of Oxford</td>
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<td>A classic problem of elasticity is to determine the possible equilibria of a planet modelled as a homogeneous compressible spherical elastic body subject to its own gravitational field. In the absence of gravity the initial radius is given and the density is constant. With gravity and for small planets, the elastic deformations are small enough so that the spherical equilibria can be readily obtained by using the theory of linear elasticity. For larger or denser planets, large deformations are possible and surprising behaviours emerge as will be revealed during this talk.</td>
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<td><strong>On the Millennium Bridge Synchronisation Myth</strong></td>
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<td><strong>Alan R Champneys, Igor Belykh, Kevin Daley, John Macdonald</strong></td>
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<td>¹University of Bristol, United Kingdom; ²Georgia State University</td>
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<td>The pedestrian-induced lateral oscillation of London's Millennium bridge on the day it opened in 2000 has become a much cited paradigm of an instability caused by phase synchronization of coupled oscillators. However, a closer examination of subsequent theoretical studies and experimental observations have brought this interpretation into question. To elucidate the true cause of instability, we study a variety of models in which each pedestrian is represented by a simplified biomechanically-inspired two-legged inverted pendulum. The key finding is that synchronization between individual pedestrians is not a necessary ingredient of instability onset. Instead, the side-to-side pedestrian motion should on average lag that of the bridge oscillation by a fraction of a cycle. Using a multi-scale asymptotic analysis, we derive a simple general criterion for bridge instability based on the notion of effective negative damping. This criterion suggests that the initiation of wobbling is not accompanied by crowd synchrony and crowd synchrony is a consequence but not the cause of bridge instability.</td>
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<td><strong>Moving-boundary problems in tissue growth</strong></td>
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<td><strong>John King</strong></td>
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<td>The growth of biological tissue is significant for both health (e.g. tissue engineering) and disease (e.g. cancer). Some simple mathematical models relevant to the macroscale (i.e. at the tissue level) will be derived by asymptotic approaches and some of their properties outlined.</td>
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<td><strong>Adaptive methods for data assimilation</strong></td>
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Christopher Budd
University of Bath, United Kingdom

Data assimilation is an essential part of modern numerical weather prediction (NWP) leading to significantly more accurate forecasts. However, a frequent problem in predicting fog or other phenomena arises from a misinterpretation of the boundary-layer structure in the assimilation procedure due to inappropriate background-error covariances. In particular features either side of a boundary layer may be falsely correlated with each other. One way to overcome this is to use an adaptive procedure in which the local computational mesh close to the boundary layer is refined. This prevents such false correlations in the data. I will show how this can be done efficiently, in real time and on large meteorological data sets, by using an adaptive mesh algorithm. This algorithm in turn relies on the use of optimal transport methods, which give a robust and fast means of performing the adaptivity. The result is a significant improvement in weather forecasting accuracy, at little extra computational cost. This is joint work with Mike Cullen and Chiara Piccolo at the UK Met Office.

11:30am - 12:00pm

Optimal Transport for Signal and Image Analysis
Soheil Kolouri
HRL Laboratories, LLC, United States of America

In this talk I will present a set of image analysis tools based on the mathematics of optimal transport problem, which can be used for a variety of biomedical imaging applications. In addition to providing basic theory relating to optimal mass transport, I will describe the recent development of image transforms with well-defined forward and inverse operations that have demonstrable advantages over classic image transforms (e.g. Fourier, wavelet, Radon). Finally, I will review the applications of these methods in image modeling, statistical analysis, classification, and inverse problems.

12:00pm - 12:30pm

Sinkhorn Divergences: Bridging the gap between Optimal Transport and MMD
Aude Genevay
Ecole Normale Supérieure, France

Sinkhorn Divergences, based on entropy-regularized OT, were first introduced as a solution to the computational burden of OT. However, this family of losses interpolates between OT (no regularization) and MMD (infinite regularization). This property is also true in terms of sample complexity, since regularizing OT breaks the curse of dimensionality. We will illustrate these theoretical claims on a set of learning problems which consist in learning a distribution from samples.

11:00am - 12:30pm

Minisymposium 6B: Shape changes in Soft and Biological Solids
Session Chair: Matteo Taffetani

11:00am - 11:30am

Large strain elasticity: geometry, instability and brains.
John Biggins
Cambridge University, United Kingdom

We are all familiar with the prototypical elastic instability: the buckling of a slender column under a compressive load. Soft elastic solids, such as rubbers, gels, and biological tissues, are united by their ability to sustain very large shape changes, and consequently undergo a range of more exotic elastic instabilities underpinned by the non-linear geometry of large strains. I will discuss several such instabilities, including fingering in soft solid layers under tension, beading in solid cylinders subject to surface tension, and a brand new "peristaltic" instability in inflated cylindrical channels. In the second half of the talk, I will discuss the buckling of a growing layer adhered to a soft substrate. I will argue on symmetry grounds that such buckling will inevitably produce patterns of hexagonal dents near threshold, and then make a biological case that this buckling process leads to the folded shape of the human brain.

11:30am - 12:00pm

Wrinkling instabilities in soft dielectric plates
Hannah Conroy Broderick
National University of Ireland, Galway, Ireland

Dielectric materials are smart materials that deform elastically in the presence of an electric field. They have potential applications in devices such as artificial muscles and soft robotics, where there is demand for materials that can undergo repeated large deformations.

We show that a smooth giant voltage actuation of soft dielectric plates is not easily obtained in practice. In principle one can exploit, through pre-deformation, the snap-through behaviour of the voltage-control loading curve to deliver a large stretch prior to electric breakdown. However, we demonstrate that even in this favourable scenario, the soft dielectric is likely to first encounter the plate wrinkling phenomenon, as modelled by the onset of small-amplitude sinusoidal perturbations on its faces.

We also investigate the case of a soft dielectric plate deformed by the coupled effects of a mechanical pre-stress applied on its lateral faces and an electric field applied through its thickness under charge-controlled actuation, where the electric field is created by spraying charges on the major faces of the plate. Although in practice this mode of actuation is harder to achieve than a voltage-driven deformation, here we find that it turns out to be much more stable in theory. We show that the geometric instability associated with the formation of small-amplitude wrinkles on the faces of the plate that arises under voltage control does not
thin liquid films are ubiquitous in natural phenomena and technological applications. They have been extensively studied via deterministic hydrodynamic equations, but thermal fluctuations often play a crucial role that needs to be understood. An example of this is dewetting, which involves the rupture of a thin liquid film and the formation of droplets. Such a process is thermally activated and requires fluctuations to be taken into account self-consistently. In this talk we present an analytical and numerical study of a stochastic thin-film equation derived from first principles. Following a brief review of the derivation, we scrutinise the behaviour of the equation in the limit of perfectly correlated noise along the wall-normal direction, as opposed to the perfectly uncorrelated limit studied by Grün et al. (J Stat Phys 122(6):1261–1291, 2006). We also present a numerical scheme based on a spectral collocation method, which is then utilised to simulate the stochastic thin-film equation. This scheme seems to be very convenient for numerical studies of the stochastic thin-film equation, since it makes it easier to select the frequency modes of the noise (following the spirit of the long-wave approximation). With our numerical scheme we explore the fluctuating dynamics of the thin film and the behaviour of its free energy in the vicinity of rupture. Finally, we study the effect of the noise intensity on the rupture time, using a large number of sample paths as compared to previous studies.

11:30am - 12:00pm

Instability, Rupture and Fluctuations in Thin Liquid Films: Theory and Computations
Rishabh Gvalani, Miguel Duran-Olivencia, Serafim Kalliadasis, Grigorios Pavliotis
Imperial College London, United Kingdom

Thin liquid films are ubiquitous in natural phenomena and technological applications. They have been extensively studied via deterministic hydrodynamic equations, but thermal fluctuations often play a crucial role that needs to be understood. An example of this is dewetting, which involves the rupture of a thin liquid film and the formation of droplets. Such a process is thermally activated and requires fluctuations to be taken into account self-consistently. In this talk we present an analytical and numerical study of a stochastic thin-film equation derived from first principles. Following a brief review of the derivation, we scrutinise the behaviour of the equation in the limit of perfectly correlated noise along the wall-normal direction, as opposed to the perfectly uncorrelated limit studied by Grün et al. (J Stat Phys 122(6):1261–1291, 2006). We also present a numerical scheme based on a spectral collocation method, which is then utilised to simulate the stochastic thin-film equation. This scheme seems to be very convenient for numerical studies of the stochastic thin-film equation, since it makes it easier to select the frequency modes of the noise (following the spirit of the long-wave approximation). With our numerical scheme we explore the fluctuating dynamics of the thin film and the behaviour of its free energy in the vicinity of rupture. Finally, we study the effect of the noise intensity on the rupture time, using a large number of sample paths as compared to previous studies.

12:00pm - 12:30pm

Is biological growth driven by stress or strain?
Alexander Erlich1, Gareth W. Jones2, Derek E. Moulton3, Alain Goriely2
1Laboratoire Interdisciplinaire de Physique (LIPhy), Université Grenoble Alpes, CNRS, Grenoble 38000, France; 2School of Mathematics, University of Manchester, Oxford Road, Manchester M13 9PL, UK; 3Mathematical Institute, University of Oxford, Andrew Wiles Building, Woodstock Road, Oxford OX2 6GG, UK

Cell growth is influenced by local mechanical cues. Locally, this leads to a mechanically heterogeneous environment as cells pull and push their neighbours in a cell network. However, at the tissue level, the cell network is remarkably robust, as it is not easily perturbed by changes in the mechanical environment or the network connectivity. Through a simple network model, we are able to link global tissue structure (i.e. the cell network topology) with local growth mechanisms (growth laws). We investigate two frequently used growth laws, termed stress-driven and strain-driven growth. We find that networks with predominantly series connections are highly likely to have underlying stress-driven growth, and networks with predominantly parallel connections are likely strain-driven.

11:00am - 11:30am

Minisymposium 13A: Fluctuating Hydrodynamics
Session Chair: James Edward Sprittles
Session Chair: Serafim Kalliadasis

11:00am - 12:30pm

Contributed Talks 28: Industrial modelling 3
Session Chair: Carl A Whitfield

11:00am - 11:20am

Modelling the Hydriding of Uranium for Nuclear Waste Storage Applications
After use in nuclear reactors, uranium waste is usually stored in water tanks or in air in sealed concrete containers. In both cases, the metal is observed to form a protective surface layer of uranium oxide (UO₃). However, hydrogen is able to slowly diffuse through the oxide to the metal (R.M. Harker, J. Alloys Compd., 426: 106–117, 2006). Once hydrogen concentration in the metal matrix has surpassed the solid solubility limit, uranium hydride (UH₃) is produced. UH₃ tends to crumble and is pyrophoric, making it detrimental to safe waste storage (J. Glascott and I.M. Findlay, J. Alloys Compd., 649: 426-439, 2015.).

A continuum mechanics model has been developed to describe the hydriding process. The salient features of the thermoelastic, reaction-diffusion model are the diffusion of hydrogen, reaction to form UH₃, and the resultant changes in temperature, stress and expansion. A finite element method was used to obtain model solutions. Global sensitivity analysis has been performed on the system, with the view to determine the most influential parameters, and motivate appropriate reduced models.

The general nature of the model means it has the potential to be extended to include more complex features which are believed to be highly influential in the overall degradation of uranium. These include applied stresses, the addition of a surface oxide layer, and small-scale processes such as the nucleation and growth of UH₃ blisters and their later breach of the UO₃ layer.
information per time unit that can be transmitted between the different parts of the brain networks considered. I will start with the working hypothesis, presented in Ref. [1] and supported by numerical evidence, that brains might evolve based on the principle of the maximisation of their internal information flow capacity. In this regard, we have found that synchronous behaviour and information flow capacity of the evolved networks reproduce well the same behaviours observed in the brain dynamical networks of the Caenorhabditis elegans (C.elegans) soil worm and humans. Then, I will talk about the verification of our hypothesis by showing that Hindmarsh-Rose (HR) neural networks evolved with coupling strengths that maximise the information flow capacity are those with the closest graph distance to the brain networks of C.elegans and humans. Finally, I will present results from a recently published paper [2] on spectacular neural synchronisation phenomenon observed in modular neural networks such as in the C.elegans brain network, called chimera-like states. I will show that, under some assumptions, neurons of different communities of the brain network of the C.elegans soil worm equipped with HR dynamics are able to synchronise with themselves whereas others, belonging to other communities, remain essentially desynchronised, a situation that changes dynamically in time.

11:40am - 12:00pm
Shear-driven instabilities in membrane tubes
Sami Cameron Al-izz1, Pierre Sens2, Matthew Simon Turner1
1University of Warwick, United Kingdom; 2Institut Curie, France

The scission of membrane tubes is a process vital to many pathways of inter-cellular transport, including endocytosis and mitochondrial fission. Motivated by the mechanics of Dynamin-mediated membrane tube fission we analyse the stability of fluid membrane tubes subjected to shear flow in azimuthal direction, driven by some active torque at the boundary. We find a novel helical instability driven by the membrane shear flow which has its onset at shear rates that are physiologically accessible under the action of Dynamin and could also be probed using in-vitro experiments on GUVs using magnetic tweezers. We discuss how such an instability may play a role in the mechanism for Dynamin-mediated membrane tube fission.

12:00pm - 12:20pm
Which head is ahead: Two stochastic models of intracellular transport, and an experiment
Gleb Zhelezov, Lyubov Chumakova
University of Edinburgh, United Kingdom

Cells have a complex internal structure of macromolecules that requires regular transport of organelles to biologically-relevant locations. Such targeted transport cannot be efficiently accomplished by passive diffusion; instead, the cell relies on molecular motors moving along an ever-shifting network of polymers (called microtubules) to deliver these important cargoes. We present a stochastic model for a molecular motor stepping along an inhomogenous bundle of microtubules, as well as a simplified model that’s simpler to analyse. Using these models, we investigate how the preferred stepping direction of the motor (parallel or antiparallel to the microtubule growth, corresponding to kinesin and dynein motor families) quantitatively and qualitatively affects the cargo delivery. Finally, we make some predictions on which type of motor is responsible for which type of cargo, and present some supporting experimental findings, due to Victor Alfred and Natalia Bulgakova (University of Sheffield).

11:00am - 12:30pm
Contributed Talks 6: Fluids 3
CB 4.8
Session Chair: Nicola Bailey

11:00am - 11:20am
Chiral transfer of angular momentum
Henry Keith Moffatt
University of Cambridge, United Kingdom

Suppose that viscous fluid is contained in the space between a fixed sphere S_2 and an interior sphere S_1 which moves with time-periodic velocity \( \mathbf{U}(t) \) and angular velocity \( \mathbf{\Omega}(t) \), with \( \langle \mathbf{U}(t) \rangle = \langle \mathbf{\Omega}(t) \rangle = 0 \). It will be shown that, provided this motion is chiral in a manner to be described, it can drive a flow that exerts a non-zero torque on S_2. Thus, mean angular momentum can be generated through this mechanism. In this sense, the effect is analogous to the MHD alpha-effect in dynamo theory. (This work is in collaboration with V.A.Vladimirov.)

11:20am - 11:40am
Euler-Poincare variational principles for wave-structure-fluid interactions
Hamid Alemi Ardakani
University of Exeter, United Kingdom

A variational principle is derived for the motion of a rigid body dynamically coupled to its interior fluid sloshing in three dimensional rotating and translating coordinates. The fluid is assumed to be inviscid and incompressible. The Euler-Poincare reduction framework of rigid body dynamics is adapted to derive the coupled PDE system for the angular momentum and linear momentum of the rigid body and for the motion of the interior fluid relative to the body coordinate system attached to the moving rigid body. The variational principle is extended to the problem of interactions between gravity-driven potential flow water waves and a freely floating rigid body dynamically coupled to its interior fluid motion in three dimensions.

11:40am - 12:00pm
Centrifugally Induced Interfacial Instabilities in a circular domain
The phenomenon of interfacial instability has been of growing interest since the initial work presented by Lord Rayleigh in his 1882 paper [1] concerning a dense incompressible fluid being supported by a less dense incompressible fluid. The importance of such instabilities is present when understanding multi-scale flows within many areas of research, from the small scale modelling of Inertial Confinement Fusion (ICF) [2] to the very large scale modelling of bubbles rising in galaxy cluster cooling flows [3, 4]. An example of such an instability is when milk is poured into black tea and we are able to see an interfacial boundary between the hot water and milk. The boundary is a good example of a density-stratified medium exhibiting a growing instability. Here we follow earlier work [5] by experimentally and theoretically investigating a circular interface between two concentric fluid layers of differing density in a circular domain. The objective is to investigate how instabilities on the interface grow when they are driven by a centrifugal, rather than gravitational, force. Hence, the whole system is rotated about its axis of symmetry. The geometry of the flow domain imposes significant technical difficulties in the initial experimental setup of the fluid layers. The fluids are separated uniformly using a strong externally applied magnetic field. The instability is then initiated by rapidly changing the applied magnet field. A linear perturbation theory to the base flow allows us to provide certain stability criteria.


12:00pm - 12:20pm
Characteristics of a Fluid Lubricated Bearing with Random External Forcing
Nicola Bailey1, Stephen Hibberd2, Michael Tretyakov2
1Department of Mechanical Engineering, University of Bath, United Kingdom; 2Faculty of Mathematical Sciences, University of Nottingham, United Kingdom

Advancements in fluid lubricated bearing and seal technology are driven by ongoing developments in industrial applications. Increasingly aero-engine technology is characterised by requiring smaller clearances and lower frictional losses, while providing improvements in efficiency and reliability. An essential consideration is that of external loading and disturbances felt by the bearing or seal from the local environment which may act to destabilise it. A fluid lubricated bearing, comprising a pair of parallel or tapered coaxial axisymmetric rotating and stationary components separated by a thin fluid film, is examined under external loading. One challenge is to minimise the fluid film between the bearing faces, to improve the efficiency of the bearing, whilst ensuring that contact between the faces can be prevented even under large disturbances. This could result in wear and lead to a possible catastrophic bearing failure, thus decreasing the reliability of the bearing. Therefore, it is necessary to have a comprehensive understanding of the bearing characteristics and essential to quantify the effect of external forces on its behaviour.

A modified Reynolds equation is derived for the pressurised fluid flow using an axisymmetric lubrication approximation and is coupled to the axial motion of the bearing faces, modelled as spring-mass-damper systems, through the axial force exerted on the bearing faces by the fluid film. Random external forces are imposed on the bearing to examine the possibility of contact between the bearing faces and bearing life span to ensure safe and reliable operation.

Results can inform bearing design, identify constraints on the operating conditions for safe and reliable behaviour and give an indication of the average lifetime of a bearing.

11:00am - 12:30pm
CB 3.11
Minisymposium 12A: Modern Approaches to Inverse Problems
Session Chair: Matthias J Ehrhardt

11:00am - 11:30am
MAP estimators and posterior consistency for Bayesian inverse problems for functions
Masoumeh Dashti
University of Sussex, United Kingdom
We consider the inverse problem of recovering an unknown functional parameter from noisy and indirect observations. We adopt a Bayesian approach, and show some results on characterisation of the modes of the posterior measure. We also discuss some posterior consistency results.
This is based on joint works with S. Agapiou, M.Burger and T. Helin.

11:30am - 12:00pm
Sparse recovery from subsampled random convolutions
Holger Rauhut
RWTH Aachen University, Germany
Compressive sensing predicts that sparse vectors can be recovered from incomplete linear measurements with efficient algorithms in a stable way. While many theoretical results work with Gaussian random measurement matrices, practical applications usually demand for structure. The talk covers the particular case of structured random measurements defined via convolution with a random vector and subsampling (deterministic or random as well). We will give an overview on the corresponding theory and will cover also recent results concerning recovery from one-bit measurements arising in quantized compressive sensing. Based on joint works with Felix Krahmer, Shahar Mendelson, Sjoerd Dirksen and Hans-Christian Jung.

12:00pm - 12:30pm
**Projection Methods, Superiorization and Applications**

**Aviv Gibali**  
ORT Braude College, Israel

Projection methods are iterative algorithms that use projections onto sets while relying on the general principle that when a family of sets is present, then projections onto the given individual sets are easier to perform than projections onto other sets that are derived from the given individual sets. Their robustness, low computational effort and their ability to handle huge-size problems make them very useful for many convex and non-convex real-world problems such as Image Reconstruction, Intensity-Modulated Radiation Therapy (IMRT) Treatment Planning as well as Sudoku and 8 Queens Puzzle.

The Superiorization Methodology is a heuristic tool and its goal is to find certain good, or superior, solutions to feasibility and optimization problems. In many scenarios, solving the full problem can be rather demanding from the computational point of view, but solving part of it, say the feasibility part is, often, less demanding.

In recent years “superiorized” projection methods and other iterative methods have been developed and applied successfully to feasibility, single and multi-objective optimization.

In this talk I will provide an overview on the above concepts, present several theoretical and practical results and also potential direction for future research.

11:00am - 11:30am
**Contributed Talks 34: Nonlinear waves**

**Session Chair: Thibault Congy**

**11:00am - 11:20am**

**Early stage of integrable turbulence in 1D NLS equation: the semi-classical approach to statistics**

**Giacomo Roberti**¹, Gennady El², Stephane Randoux³, Pierre Suret²

¹Northumbria University, NE1 8ST - Department of Mathematics, Physics and Electrical Engineering, Newcastle upon Tyne, UK; ²Univ. Lille, CNRS, UMR 8523 - Physique des Lasers Atomes et Molécules (PHLAM), F-59000 Lille, France

The concept of integrable turbulence introduced by Zakharov [1] has been recently recognised as a novel theoretical paradigm of major importance for a broad range of physical applications from photonics to oceanography. One of the applications of the integrable turbulence theory is the statistical description of the appearance of rogue waves.

We consider the evolution of an initial partially coherent wave field with Gaussian statistics in the framework of the integrable one-dimensional nonlinear Schrödinger equation (1D-NLSE), and we analyse the normalized fourth order moment of the field’s amplitude, which characterises the “tailedness” of the probability density function (PDF). The relation between this statistical quantity and the spectral width of the field has been recently provided in Onorato et al. [2], however, it requires the spectral width knowledge at each step in time.

In our work, thanks to the combination of tools from the wave turbulence theory and the semi-classical theory of 1D-NLSE, we derive for the first time an analytical formula for the short time evolution of the fourth order moment as a function of the statistical characteristics of the initial condition. This formula provides a quantitative description of the appearance of the “heavy” ("low") tail of the PDF in the focusing (defocusing) regime of the 1D-NLS at the initial stage of the development of integrable turbulence, and our theoretical predictions exhibit a good agreement with the numerical simulations.


**11:20am - 11:40am**

**Nonlinear Schrödinger equations and the universal description of dispersive shock wave structure**

**Thibault Congy**¹, Gennady El², Mark Hoefer³, Michael Shearer³

¹Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle upon Tyne, UK; ²Department of Applied Mathematics, University of Colorado, Boulder, Colorado, USA; ³Department of Mathematics, North Carolina State University, Raleigh, North Carolina, USA

A dispersive shock wave (DSW) is an expanding, modulated nonlinear wavetrain that connects two disparate hydrodynamic states, and can be viewed as a dispersive counterpart to the dissipative, classical shock. DSWs have raised a lot of interest in the recent years, due to the growing recognition of their fundamental nature and ubiquity in physical applications, examples being found in oceanography, meteorology, geophysics, nonlinear optics, plasma physics and condensed matter physics. Although well-established methods, such as the Whitham modulation theory, have proved particularly effective for the determination of DSW solutions of certain nonlinear wave equations, a universal description of these objects is still lacking.
The nonlinear Schrödinger (NLS) equation and the Whitham modulation equations both describe slowly varying, locally periodic nonlinear wavetrains, albeit in differing amplitude-frequency domains. Taking advantage of the overlapping asymptotic regime that applies to both the NLS and Whitham modulation descriptions, we developed a universal analytical description of DSWs generated in Riemann problems for a broad class of integrable and nonintegrable nonlinear dispersive equations. The proposed method extends DSW fitting theory that prescribes the motion of a DSW’s edges into the DSW’s interior, that is, this work reveals the DSW structure. I will present this new method and illustrate its efficacy by considering various physically relevant examples.

11:40am - 12:00pm
Generalised Coupled Nonlinear Schrodinger Equation and its Applications to Nonlinear Mechanical Topological Insulators
David Snee, Yi-Ping Ma
Northumbria University, United Kingdom

We show theoretically that the classical 1D nonlinear Schrödinger (NLS) and coupled nonlinear Schrodinger (CNLS) equations govern the envelope(s) of localised and unidirectional nonlinear travelling edge waves in a 2D mechanical topological insulator (MTI). The MTI consists of a collection of pendula with weak Duffing nonlinearity connected by linear springs and it is found that the NLS and CNLS respectively describe the unimodal and bimodal properties of the nonlinear system.

The theoretical predictions from the 1D NLS are confirmed by numerical simulations of the original 2D system for various types of travelling waves and rogue waves. The governing bimodal CNLS is found to be non-integrable by nature and as such we consider new solutions by exploring the spatial dynamics of the reduced generalised travelling wave ODE. Such solutions include pinned travelling fronts.

In the original 2D MTI, as a result of topological protection, the edge solitons persist over long time intervals and through irregular boundaries. The existence of topologically protected edge solitons may have significant implications on the design of acoustic devices, with potential applications to collision-based computing.

12:30pm - 1:30pm
Lunch and Poster Session 2
Foyer, Level 1
Session Chair: Tim Rogers
Session Chair: Apala Majumdar

1:30pm - 3:00pm
Minisymposium 9B: Dynamics of Complex Contagions
CB 3.5
Session Chair: Sam Moore
Session Chair: Tim Rogers

1:30pm - 2:00pm
From interdependent percolation to cooperative contagion processes on multilayer networks
Ginestra Bianconi
Queen Mary University London, United Kingdom

Multilayer networks describe systems formed by several networks that interact which each other and affects dynamical processes determining novel critical phenomena that cannot be captured by considering layers taken in isolation.

In this talk I will discuss recent results on interdependent percolation on multiplex networks and their connection with cooperative epidemic processes on the same structure revealing novel dynamical processes leading to abrupt phase transitions.

2:00pm - 2:30pm
Infection speed on Networks
Sam Moore
University of Bath, United Kingdom

An important question when studying infections on networks is how quickly the infection spreads away from its source. In this talk I show how we have calculated this quantity on a sparse random graph and demonstrate some additional connected results.

2:30pm - 3:00pm
Impact of complexity of contagion and contact on spreading dynamics
Thomas House
University of Manchester, United Kingdom

Mark Twain is often credited (perhaps incorrectly) with the statement: “a lie can travel halfway around the world while the truth is still putting on its shoes”. While the Black Death spread through Medieval Europe in a diffusive manner over years, modern pandemics jump between continents in days and a “viral” tweet can be spread across the whole world in seconds. In this talk, I will present mathematics that deals with the two main posited causes of this acceleration of transmission: first, complexity of the contagion process due to social influence or biological phenomena; and secondly the complexity and higher interconnectedness of the contact networks on which the spreading occurs.

1:30pm - 3:00pm
Minisymposium 11B: New Perspectives and Challenges at the Junction of Modelling and Applications
CB 4.1
Session Chair: Apala Majumdar

1:30pm - 2:00pm
Likely instabilities in stochastic hyperelastic solids
L. Angela Mihai
Cardiff University, United Kingdom

Nonlinear elasticity has been an active topic of fundamental and applied research for several decades. However, despite numerous developments and considerable attention it has received, there are important issues that remain unresolved, and many aspects still elude us. In particular, the quantification of uncertainties in material parameters and responses resulting from incomplete information remain largely unexplored. In this talk, I will consider stochastic hyperelastic material models described by a strain-energy density where the parameters are random variables characterised by probability density functions. These models, which are constructed through a Bayesian identification procedure, rely on the notion of entropy (or uncertainty) and on the maximum entropy principle, and enable the propagation of uncertainties from input data to output quantities of interest. To demonstrate the effect of probabilistic model parameters on predicted mechanical responses, selected specific problems include the cavitation and nonlinear oscillatory motion of a sphere under uniform tensile dead loads.

2:00pm - 2:30pm
Quantization, chaotic dynamics and emergent statistics of a hydrodynamic pilot-wave system
Matthew Durey1,2, Paul A. Milewski2, John W. M. Bush1
1Massachusetts Institute of Technology, United States of America; 2University of Bath, United Kingdom

A droplet may ‘walk’ along the surface of a vertically vibrating fluid bath, propelled at each impact by the Faraday waves generated by all prior impacts. The longevity of this ‘path memory’ increases with the amplitude of the vibrational forcing, yielding instabilities in the system and the onset of chaos. This hydrodynamic pilot-wave system exhibits many features that were previously thought to be exclusive to the quantum realm, such as unpredictable tunnelling, emergent statistics, and quantized droplet dynamics.

From first principles, we derive a discrete-time iterative map to explore the pilot-wave dynamics when the droplet is subjected to a harmonic potential. In the long-path-memory limit we see the emergence of wave-like statistics, random-walk-like dynamics, and the presence of an effective potential induced by the long-lived Faraday waves. Based on our observations of the deterministic dynamics, we propose a simple stochastic model for the pilot-wave system.

2:30pm - 3:00pm
Active and passive driving in liquid crystal devices
Oliver Whitehead1, Ian M. Griffiths1, Apala Majumdar2, Colin P. Please1
1University of Oxford, United Kingdom; 2University of Bath, United Kingdom

Liquid crystal devices form a continually growing multi-billion-dollar industry which has garnered an increased level of academic interest in recent years. Several models for these devices have been well studied including the Ericksen-Leslie model for nematic liquid crystals. In this talk, I will present an extension of this model to more modern active-matrix liquid-crystal displays.

1:30pm - 3:00pm
Contributed Talks 19: Cardiac dynamics
Session Chair: Hao Gao

1:30pm - 1:50pm
Inter-subject variability in rabbit ventricular myocytes and their responses to IKr block
Muhamad Hitghudin Noor Aziz1, Francis Burton2, Godfrey Smith2, Radostin D. Simitev1
1School of Mathematics and Statistics, University of Glasgow, UK; 2Institute of Cardiovascular and Medical Sciences, University of Glasgow, UK

Cell variability in cardiac electrophysiology occurs due to the variability in ion channel densities and in turn leads to various action potential morphologies (AP) even under control conditions. We conducted an experimental and a computational study on populations of rabbit cardiomyocytes in order to investigate the effects of variability in action potentials and the cellular response to drug blocking of the rapid component of the delayed rectifier potassium current (IKr). 272 AP recordings from rabbit’s hearts were used to construct a population of rabbit ventricular models with normal APs and a wide range of ion channel densities. We then applied 30nM concentration of dofetilide on the cells at pacing rate of 2Hz and observed the actions of the drug block. We found that the electrophysiological of the cells react differently to the drug and we classified the AP responses into three categories which are 1) action potential duration (APD) prolongation, 2) hyper-response and 3) early after-depolarisation (EAD). From our work, we also found that in cells where L-type calcium current is high, reduction of IKr can cause the cellular repolarization abnormalities.

1:50pm - 2:10pm
Effects of myofibre architecture on biventricular biomechanics: a simulation study
Debao Guan1, Jiang Yao2, Xiaoyu Luo1, Hao Gao1
1School of Mathematics and Statistics, University of Glasgow, UK; 2Simula Virtual Human Modelling, Dassault Systemes Simulia Corp., USA

Cardiac diseases remain a major public healthy burden, especially the adverse remodelling of cardiac function after acute myocardial infarction (MI). Studies have demonstrated that mechanical stresses and strains in myocardium can have great effects on pathological processes. The three-dimensional (3-D) spatial architecture of myofibres play a very important role in heart function, such as influencing electrical propagation, myocardial expansion in diastole and contraction in systole. To include myofibres into the
computational models, two different approaches have been widely used in the literature, one approach is directly mapping myofibres from ex vivo datasets to the computational models, for example the model reconstructed directly from diffusion-tensor magnetic resonance (DT-MRI) datasets or using atlas-based methods to warp the DT-MRI data into the models. The other approach is the rule-based method (RBM) in which myofibres rotate from endocardium to epicardium with prescribed angles, varied linearly in most of studies. This study develops a 3D neonatal bi-ventricle porcine model to compare ex vivo DT-MRI myofiber architecture based on large deformation diffeomorphic metric mapping (LDDMM) framework with two different simplifications based on a rule-based approach. The first simplification uses AHA17 segments to reconstruct myofibres with different fibre angles at each segment, a further simplification is made by assigning the same fibre rotation angles in the whole ventricle. Different approximations of myofibre architecture are compared in terms of cardiac pump function. Results show that using realistic myofibre architecture can produce better cardiac output, higher ejection fraction and larger apical twist compared to the simplified rule-based myofibres, even though they all are derived from the same DT-MRI dataset. Therefore, it is necessary to incorporate a realistic myofibre architecture if personalized ventricular models are needed.

2:10pm - 2:30pm

Challenges in Variability and Uncertainty Quantification for Ion Channel Modelling

Chon Lok Lei1, Michael Clerx1, David J Gavaghan1, Liudmila Polonchuk2, Ken Wang2, Gary R Mirams3

1University of Oxford, Oxford, United Kingdom; 2F. Hoffmann-La Roche Ltd., Basel, Switzerland; 3University of Nottingham, Nottingham, United Kingdom

Biophysical models are subject to parameter uncertainties, but also to variability between measurements and uncertainty in the model structure. Such variability together with limited uncertainty quantification causes reproducibility issues. Here we show methods and challenges in quantifying variability and uncertainty in parameters for a cardiac potassium channel model.

Designing high information-content experiments helps us to parameterise models with short training experiments, whilst leaving time to do independent validation experiments which help with model validation and eventually model selection. We based our analysis on 50 experimental recordings and used methods such as hierarchical Bayesian modelling to quantify the variability and uncertainty between measurements and the correlation between model parameters.

This study raise questions about how best to account for parameter correlations, model variability, model discrepancy and uncertainty when using these models to make real world decisions, how to design the best training and validation experiments, and how to put correlated variability and uncertainty bounds on our model predictions.

2:30pm - 2:50pm

Mathematical Modelling of Coupled Myocytes and Fibroblasts with Myocardial Infarction scars.

Peter Mortensen1, Radostin Simitev1, Godfrey Smith2, Hao Gao1

1University of Glasgow, School of Mathematics and Statistics; 2University of Glasgow, Institute of Cardiovascular and Medical Sciences

The heart beat is controlled by an electrical wave that propagates with a particular pattern. This pattern allows blood to be pumped through the heart with maximum efficiency. However, when a myocardial infarction damages the muscle tissue, this pattern is interrupted, leading to arrhythmia and heart failure. This is due to the changes in the cardiac tissue caused by the damage, specifically death of myocytes and increase of fibroblasts and collagen, in a process called fibrosis.

Current work couples existing models of myocytes and fibroblasts to create a more comprehensive electrophysiological model of infarcted cardiac tissue. The models being used are for human atrial myocytes (by Courtemanche et al [1]) and for rabbit ventricular myocytes (by Weiss et al [2]). Both models are coupled with a fibroblast electrophysiology model by Morgan et al [3]. By varying the number of fibroblasts and myocytes that are coupled we can begin to create a model of the fibrosis that converts a region of healthy tissue to an myocardial infarction scar. Finite element methods are used to solve this model and explore the numerous effects of the coupling on the propagation of electrical properties in cardiac tissues in 1D strips and 3D slabs.

Currently, the simulations produce contour plots for key properties such as activation times, calcium concentration and action potential duration. We can also determine the critical ratio of the number of fibroblasts coupled to a myocyte at which action potentials fail to propagate. Future work will involve adapting the fibroblast model to reflect the changes that fibroblasts undergo when they become active to begin the fibrosis process. Also, we will use more realistic geometries as well as coupling these models with models of muscle contraction as well as using more realistic geometries.

Acknowledgements: SofTMech centre for Multiscale Soft Tissue Mechanics

1:30pm - 3:00pm

CB 3.16

Minisymposium 15: Mathematical Neuroscience

Session Chair: Stephen Coombes
Session Chair: Kyle Wedgwood

1:30pm - 2:00pm

Understanding sensory induced hallucinations: from neural fields to amplitude equations

Stephen Coombes1, Abigail Cocks1, Alan Johnston2, Daniele Avitabile3

1School of Mathematical Sciences, University of Nottingham, United Kingdom; 2School of Psychology, University of Nottingham, United Kingdom

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Explorations of visual hallucinations, such as in [1], show that annular rings with a background flicker can induce visual hallucinations in humans that take the form of radial fan shapes and vice versa. The well-known retino-cortical map tells us that the corresponding patterns of neural activity in the primary visual cortex for rings and arms in the retina are orthogonal stripe patterns. The implication is that cortical forcing by spatially periodic input can excite orthogonal modes of neural activity. To understand this phenomenon we consider a simple planar neural field model, that supports a Turing instability to a spatially periodic pattern, and then include a further component of spatial drive. By utilising a weakly nonlinear multiple-scales analysis we determine the relevant amplitude equations for understanding pattern formation. These are found to be reminiscent of the Newell-Whitehead-Segel equations, generalised to include the effect of spatial periodic forcing [2]. In turn we use these to uncover the parameter regimes which favour the excitation of patterns orthogonal to sensory drive, and thus shed light on the original psycho-physical observations in [1].


2:00pm - 2:30pm

**Dynamics of visual perception with periodically changing stimuli**

**James Rankin, Farzaneh Darki**

University of Exeter, United Kingdom

This research aims to understand the neural dynamics and mechanisms underlying perceptual bistability. This phenomenon occurs when the two eyes are presented with incompatible stimuli and perception alternates between these two stimuli. This phenomenon has been investigated in two types of experiments: 1) Traditional experiments where the stimulus is fixed, 2) Eye-swap experiments in which stimulus periodically swaps between eyes many times in a second (Logothetis & Leopold 1996). In spite of the rapid swapping between eyes perception can be stable for many seconds with specific stimulus parameter configurations. Wilson (2003) introduced a two-stage, hierarchical model to explain both types of experiment. The first stage represents monocular neurons in primary visual cortex (V1), and the second stage represents binocular neurons in higher cortical areas. Wilson's model can explain maintained stimulus dominance across eye swaps. However, this and other presented competition models have been only studied with bifurcation analysis for fixed inputs and different dynamical behaviour that can occur with periodically forcing inputs were not investigated yet. To fully explain this phenomenon, we need to understand the bifurcations occurring between different states: perception following the stimulus swaps and perception being stable for many seconds. We reveal a rich organisation of complex dynamical behaviour including relaxation oscillations, mixed-mode oscillations and a period-doubling cascade to chaos. We further explore how these dynamics interact with periodic forcing as in eye-swap experiments.

2:30pm - 3:00pm

**The bump's in the waves: spatiotemporal patterns in spiking neural networks**

**Kyle CA Wedgwood, Daniele Avitabile**

University of Exeter, United Kingdom

Certain neural systems show computation through patterned activity: persistent localised activity, in the form of bumps, has been linked to working memory, whilst the propagation of activity in the form of waves has been associated with binocular rivalry tasks. Individual neurons typically exhibit an all-or-nothing response, dependent on the summation of signals they receive from the rest of the network. This fact, coupled with the desire to understand coherent patterns of activity across the network has resulted in the widespread use of non-smooth neural models that greatly simplify the complex dynamics of individual cells. Whilst these descriptions often provide tractable models of neural tissue, their non-smooth nature presents its own mathematical challenges. We will show how localised bumps of activity and travelling waves are generated in a synaptically coupled neural network and how they lose stability through bifurcations of both smooth and non-smooth type. This will be done through the specification of a voltage operator that maps firing sets, which mark which neurons at a given time are spiking, to full spatiotemporal profiles. We will show that such an operator facilitates the construction of travelling wave solutions with arbitrarily many threshold events and further demonstrate that the speed of these waves is strongly dependent on the number of spiking neurons. This observation and examination of trajectories and their linear stability provide evidence that bumps, and deterministic meandering bumps: are a form of spatiotemporal chaos in which the dynamics visit a large number of unstable &nbsp;localised travelling waves.

1:30pm - 2:00pm

**Minisymposium 8B: The multiphysics of liquid films, drops, and fibers**

Session Chair: Matthew G. Hennessy

1:30pm - 2:00pm

**Deformation of liquid surfaces under impinging gas jets: modelling and experiments**

**Chinasa Juliet Ojiako1, Radu Cimpeanu2, Hemaka Bandulasena3, Roger Smith1, Dmitri Tseluiko2**

1Department of Mathematical Sciences, Loughborough University, UK; 2Mathematical Institute, University of Oxford, UK; 3Department of Chemical Engineering, Loughborough University, UK

We consider liquid in a cylindrical beaker and study the deformation of its surface under the influence of an impinging gas jet that is generated by maintaining a constant gas flow rate from a stationary cylindrical tube with its axis coinciding with the axis of the beaker. Analysing such a system not only is of fundamental theoretical interest, but also of industrial importance, e.g., in metallurgical applications. The solution of the full set of governing equations is computationally expensive. Therefore, to obtain initial insight into relevant
regimes and timescales of the system, we first derive a reduced-order model (a thin-film equation) based on the long-wave assumption and on decoupling the gas problem from that for the liquid, taking into account a disjoining pressure. This is possible under suitable conditions, namely, when the liquid layer is thin and the typical liquid velocity is sufficiently smaller than that of the gas. We also perform direct numerical simulations (DNS) of the full governing equations using two different approaches, the CFD package COMSOL with the moving mesh interface and the volume-of-fluid Gerris package. The DNS are used to validate the results for the thin-film equation and also to investigate the regimes that are beyond the range of validity of this equation (e.g., when the liquid layer is thicker). We additionally compare the computational results with experiments. We find surprisingly that the thin-film equation produces good agreement with DNS and experiments even for flow conditions that are well beyond the theoretical region of the validity of this equation.

For a sufficiently thin film, we find that at relatively low gas flow rates, flow in the liquid evolves into a steady state with one recirculation region and with the interface having a cavity in the centre. At larger gas flow rates, the liquid film ruptures in the centre and dewets until reaching a steady state. We analyse the rupture time as well as the time evolution of the radius of the dry spot. For a thicker liquid layer, the flow in the liquid again evolves into a steady state at sufficiently low gas velocities. However, the number of the recirculation regions in the liquid increases as the liquid thickness increases. At higher gas flow rates, the flow in the liquid becomes unsteady with time-periodic or irregular oscillations being generated. We study the frequency and period of these oscillations and their dependence on the gas flow rate.

Finally, in addition to analysing gas jets acting on liquid surfaces, we also study gas plasma jets acting on liquid surfaces taking into account chemical kinetics. In particular, we analyse the accumulation and chemical reactions of plasma generated reactive species in the liquid and how these are affected by the flow in the liquid generated by the impinging jet. This has applications, for example, in water purification and wound treatment.

2:00pm - 2:30pm

Electrostatic control of instabilities in thick liquid layers

Alexander Wray1, Radu Cimpeanu2

1University of Strathclyde, United Kingdom; 2University of Oxford, United Kingdom

A common approach to understanding a fluid-dynamical system is that of a low-order model: a mathematically rigorous simplification of the governing equations (typically an asymptotic reduction of the Navier-Stokes equations) to a system of PDEs that are more analytically tractable. This usually relies on the identification of some disparity in length scales within the problem, such as the “aspect ratio” of a wave’s length to its height, to allow analytic simplification of the governing equations.

In non-planar situations, the curvature of the underlying substrate complicates the situation by incorporation of two additional length scales: the radii of curvature. In such situations, modelling has typically relied on some potentially prohibitive symmetry assumption, or the assumption that the substrate shape is slowly varying. We have shown in recent years that a combination of a novel set of scalings, together with the application of the method of weighted residuals, can relax these assumptions to accurately model situations where the fluid thickness is in excess of the radius of curvature.

The methodology has since been extended to cope with additional physical systems, including the leaky dielectric model for electrohydrodynamics. As a consequence, we have studied a canonical thick-flow problem: the Moffatt problem for flow on the outside of a rotating cylinder, and the control thereof using electric fields. Via comparison with Direct Numerical Simulations, we show that good accuracy can be maintained even for thick films at moderate levels of inertia. We note that the electrostatic problem is of particular interest as past approaches to such thick problems have typically requires complex nonlocal integral operators; a phenomenon we avoid entirely.

2:30pm - 3:00pm

Stability of a liquid membrane attached to the inside of a vertical cylinder

Matthew Haynes1, Eugene Benilov2

1Open University, United Kingdom; 2MACSI, University of Limerick, Ireland

We investigate the stability of a liquid membrane attached to the inside of a vertical cylinder by examining the energy functional of the system. In particular, we consider the most destabilising perturbations, which we show must be axisymmetric and construct an eigenvalue problem that indicates the stability of the membrane. The results of this method are then used to verify a bifurcation method which is able to predict neutral stability with significantly less computational work. Finally, we present the stability diagram and show that while increasing the Bond number in general acts to destabilise configurations, it stabilises a small region of the parameter space.

3:00pm - 3:30pm

Modelling finger flow wetting fronts in soils with the Richards equation and the Preisach operator

Denis P Flynn, Warren Roche, Kieran Murphy

Waterford Institute of Technology, Ireland

The unsaturated flow of water through porous media can undergo unstable wetting fronts in soils is known as finger flow. Thus named as the wetting fronts maintain an almost constant width or finger-like shape. In addition, these wetting fronts will be “remembered” by the soil as these same paths will be followed by the water in the future even when the soil has dried out.

The above behaviour is captured by the Richards equation, a PDE which models water movement in soils, which is modified to include hysteresis and dynamic non-equilibrium behaviour.
In this talk, we will present a model, where hysteresis is incorporated using the Preisach operator. The results of numerical solutions to this model will also be presented.

1:30pm - 3:30pm

Minisymposium 10B: Recent advances in PDE models describing emergent behaviour and collective dynamics

Session Chair: Bertram Düring
Session Chair: Marie-Therese Wolfram

1:30pm - 2:00pm

Boltzmann-type optimal control problems

Giacomo Albi
University of Verona, Italy

In this talk we consider a system of interacting Brownian particles. When diffusing particles interact with each other their motions are correlated, and the configuration space is of very high dimension. Often an equation for the single-particle density function (the concentration) is sought by integrating out the positions of all the others. This leads to the classic problem of closure, since the equation for the concentration so derived depends on the two-particle correlation function. We discuss two common closures, the mean-field (MFA) and the Kirkwood superposition approximations, as well as an alternative approach, which is entirely systematic, using matched asymptotic expansions (MAE). We compare the resulting (nonlinear) diffusion models with Monte Carlo simulations of the stochastic particle system, and discuss for which types of interactions (short- or long-range) each model works best.

2:00pm - 2:30pm

Proximal Methods for Mean Field Games with Local Couplings

Dante Kalise
Imperial College London, United Kingdom

We address the numerical approximation of Mean Field Games with local couplings. For power-like Hamiltonians, we consider both unconstrained and constrained stationary systems with density constraints in order to model hard congestion effects. For finite difference discretizations of the Mean Field Game system, we follow a variational approach. We prove that the aforementioned schemes can be obtained as the optimality system of suitably defined optimization problems. In order to prove the existence of solutions of the scheme with a variational argument, the monotonicity of the coupling term is not used, which allow us to recover general existence results. Next, assuming next that the coupling term is monotone, the variational problem is cast as a convex optimization problem for which we study and compare several proximal type methods. These algorithms have several interesting features, such as global convergence and stability with respect to the viscosity parameter, which can eventually be zero. We assess the performance of the methods via numerical experiments.

2:30pm - 3:00pm

Stationary States and Asymptotic Behaviours of Aggregation Models with Nonlinear Local Repulsion

Jose A Carrillo1, Yanghong Huang2, Marcus Schmidtchen1
1Imperial College London, United Kingdom; 2University of Manchester, United Kingdom

We study a nonlocal two species cross-interaction model with cross-diffusion. We compute analytical stationary states and travelling pulse solutions for a particular model in the case of attractive-attractive/repulsive-repulsive cross-interactions. We show that, as the strength of the cross-diffusivity decreases, there is a transition from adjacent solutions to completely segregated densities, and we compute the threshold analytically for attractive-repulsive cross-interactions. Other bifurcating stationary states with various coexistence components of the support are analyzed in the attractive-attractive case. We find a strong agreement between the numerically and the analytically computed steady states in these particular cases, whose main qualitative features are also present for more general potentials.

3:00pm - 3:30pm

Diffusion of particles with short-range interactions

Maria Bruna, Stephen Jonathan Chapman, Martin Robinson
University of Oxford, United Kingdom

In this talk we consider a system of interacting Brownian particles. When diffusing particles interact with each other their motions are correlated, and the configuration space is of very high dimension. Often an equation for the one-particle density function (the concentration) is sought by integrating out the positions of all the others. This leads to the classic problem of closure, since the equation for the concentration so derived depends on the two-particle correlation function. We discuss two common closures, the mean-field (MFA) and the Kirkwood superposition approximations, as well as an alternative approach, which is entirely systematic, using matched asymptotic expansions (MAE). We compare the resulting (nonlinear) diffusion models with Monte Carlo simulations of the stochastic particle system, and discuss for which types of interactions (short- or long-range) each model works best.
Modelling stochastic biological systems
Cameron Andrew Smith
University of Bath, United Kingdom

A large proportion of biological systems evolve under the influence of stochasticity. This proportion increases if we broaden the definition of stochasticity to include aspects of the dynamics which we either cannot predict, do not fully understand or choose to exclude from our explicit modelling. The degree to which stochasticity is important depends on the specifics of the biology and the questions which we would like to answer, but there are many biological systems for which stochasticity cannot simply be ignored.

Within this talk, I will introduce several biological problems, the stochastic methods that have been utilised in order to solve them, and investigate the insights that the randomness is able to yield. We will also explore how we can combine different stochastic and deterministic modelling paradigms in order to obtain methods which are both accurate and efficient.

Particle-based simulations of stochastic reaction-diffusion processes with Aboria
Martin Robinson¹, Philip Maini², Maria Bruna²
¹Department of Computer Science, University of Oxford; ²Mathematical Institute, University of Oxford

Mathematical models of transport and reactions in biological systems have been traditionally written in terms of partial differential equations (PDEs) that describe the time evolution of population-level variables. In recent years, the use of stochastic particle-based models, which keep track of the evolution of each organism in the system, has become widespread. These models provide a lot more detail than the population-based PDE models, and are able to capture and explain the particle-level (for example, molecule- or cell level) features that we are now obtaining from experiments.

The computational requirements of particle-based models, such as the efficient calculation of interactions, are challenging to implement in a way that scales well with the number of molecules and is flexible enough to handle both uniform and non-uniform particle distributions, different numbers of spatial dimensions and periodic/non-periodic boundary conditions. The majority of existing particle-based software is typically designed to suit a particular application or focused on a handful of modelling methodologies, and therefore tends not to be sufficiently generic that it can be used to implement arbitrary interactions between particles, or arbitrary coupling between particles and other PDE-based models.

In this presentation we overview Aboria (https://github.com/aboria/Aboria), a powerful and flexible C++ library for the implementation of numerical methods for particle-based models. Aboria aims to provide a general purpose library that allows the user complete control to define whatever interactions they wish on a given particle set, while implementing efficiently the difficult algorithmic aspects of particle-based methods, such as spatial data-structures, local neighbourhood searches and the calculation of long-range forces.

Equilibration times within heterogeneous crowded environments
Daniel Wilson¹, Matthew Simpson², Ruth Baker¹, Francis Woodhouse¹
¹University of Oxford, United Kingdom; ²Queensland University of Technology, Australia

Most biological processes that occur within the cell hinge upon the optimal transport of macromolecules such as proteins, nucleic acids and lipids. Transport of these macromolecules are impeded by the organelles within the cellular environment. The non-uniform placement of these organelles creates a complex geometry to which the molecules are constrained. I start by deconstructing these geometries into two region types; one where molecules move freely, and another where there are strong macromolecular crowding effects. Through reconstruction of the intracellular environment as a network, I present a mathematical framework that allows for the investigation of the transport of molecules across macroscopic spatial scales whilst accounting for heterogeneous microscopic spatial structure. Using the proposed framework, I investigate the properties of optimal networks which minimise the equilibration time of a diffusing population of molecules.

Stochastic amplification of oscillatory gene expression underlies cell differentiation during embryonic neurogenesis
Jochen Kursawe, Cerys Manning, Veronica Biga, Nancy Papalopulu
University of Manchester, United Kingdom

The control and downstream interpretation of gene expression dynamics is crucial in many biological contexts. For example, gene expression oscillations have been proposed to control the timing of cell differentiation during embryonic neurogenesis. Here, we mathematically model novel data of oscillatory gene expression dynamics in mouse embryonic spinal cord tissue. By combining mathematical modelling and quantitative experimental data we show that these dynamics can be understood as a result of stochastic amplification, where oscillations are enhanced by intrinsic noise. We show how such oscillations can be initiated by changes in biophysical parameters and consider mechanisms that may enable the downstream interpretation of dynamic gene expression. Our analysis illustrates how quantitative modelling can help unravel fundamental mechanisms of transcriptional regulation.
General Framework for Fluctuating Dynamic Density Functional Theory

Serafim Kalliadasis1, Miguel A. Duran-Olivencia1, Peter Yatsyshin1, Benjamin D. Goddard2

1Department of Chemical Engineering, Imperial College, United Kingdom; 2School of Mathematics and the Maxwell Institute for Mathematical Sciences, University of Edinburgh

We begin by discussing the derivations of the Dean-Kawasaki (DK) model for fluctuating hydrodynamics, and of (deterministic) dynamical density functional theory (DDFT). We then highlight the differences between the two formalisms, in particular focusing on the inclusion of anisotropic particles, hydrodynamic interactions (bath-mediated forces), and noise. Our main contributions are the derivation of a generalised fluctuating hydrodynamics (DK) equation and the corresponding fluctuating DDFT. Whilst the resulting equations are superficially very similar, there are, in fact, stark differences. Particular focus will be given to these differences, the question of if one can simply add noise to standard DDFTs, and the lack of particle correlations in the DK model. We conclude that our general fluctuating DDFT is the most appropriate formalism in which to study many non-equilibrium systems.

2:00pm - 2:30pm

A data-driven approach to model reduction: Deep-learning memory effects

Antonio Russo1, Miguel A. Durán-Olivencia1, Ioannis G. Kevrekidis1, Serafim Kalliadasis1

1Department of Chemical Engineering, Imperial College London, London, UK; 2Department of Chemical and Biomolecular Engineering, Applied Mathematics and Statistics, Johns Hopkins University, Baltimore, Maryland, US

Despite the immense advances and drastic improvement in computational power over the last decades, modelling the dynamics of multiscale systems, typically characterised by multiple time- and lengthscales nonlinearly interacting with each other, still represents a major computational challenge. Atomistic simulations, in particular, which have received considerable attention over the last few years, are still only applicable to small volumes and short time scales, especially for complex systems such as polymers and proteins. An alternative to direct numerical microscopic simulations is the so-called model-reduction (or coarse-graining) techniques put forward already in the 1960's aiming to bridge the microscopic and macroscopic worlds. The main idea is to go from the full set of degrees of freedom (DoF) to a reduced set of order parameters (or reaction coordinates) and obtain effective macroscopic descriptions by averaging out the microscopic information but retaining the main effects at the macroscopic level. The increasing demand of computational models capable of reproducing (or at least approximating) physical experiments have brought back to attention the model-reduction techniques. But at the same time these techniques suffer from various limitations, including unknown functions and parameters, as well as various assumptions and simplifications. In this work, we try to overcome these shortcomings by combining model reduction with modern data-analysis tools. In particular we make use of a projection-operator approach to obtain a general time-evolution equation with memory (i.e., non-Markovian) for any reduced set of coordinates of the complex system at hand. This non-Markovian dynamical equation is known as the generalised Langevin equation (GLE). In general, the memory-dependent terms appearing in the GLE depend on both the full set of DoF and the whole history of the complex system, hence making the problem intractable. We propose a data-driven solution to this issue by deep-learning the memory terms with a feedforward artificial neural network from observations of the full set of DoF. Once the GLE is completed with the neural network, we can make long-term simulations of the reduced coordinates with a significantly lower computational cost. Our methodology is tested by comparing the data-driven GLE predictions against simulations of the full system. The developed method outperforms previous approaches in terms of both efficiency and robustness, being much less sensitive to data fluctuations. We show excellent agreement between the reduced and the full system dynamics for colloidal systems and particle chains immersed in a thermal bath. The proposed methodology is also exemplified with applications from climatology and finance.

2:30pm - 3:00pm

A finite volume scheme for stochastic PDEs

Sergio P. Perez1,2, Antonio Russo1, Miguel A. Duran-Olivencia1, Peter Yatsyshin1, Jose A. Carrillo2, Serafim Kalliadasis1

1Department of Chemical Engineering, Imperial College London, United Kingdom; 2Department of Mathematics, Imperial College London, United Kingdom

The description of soft matter systems out of equilibrium requires the inclusion of fluctuations in the standard hydrodynamic equations for the average evolution of conserved quantities, such as density or linear momentum. The associated general framework was postulated phenomenologically by Landau et. al. [1], yielding what is known as Landau-Lifshitz fluctuating hydrodynamics (FH). This formalism has attracted considerable attention from the theoretical front, where a rigorous proof of the FH equations from the Hamiltonian microscopic description has only been developed recently [2]. However, the numerical applicability of the fluctuating hydrodynamics entails several challenges which still remain elusive. In particular, conservative fluctuations, i.e. stochastic fluxes under the gradient operator, need to be properly accounted for. Besides, even for the simplest limit of these equations which corresponds to the stochastic diffusion equation, the presence of a normally-distributed flux in the time-evolution equation for the density involves non-positive solutions, which are clearly unphysical. To address this issue, recent works have proposed empirical limiters which artificially modified the natural fluctuations of the system to preserve positivity [3]. This leads to a spurious contribution that might be negligible in thermodynamic-equilibrium conditions. Nevertheless, in more general scenarios, e.g. the evolution of a thermodynamically-metastable system, the spurious contribution coming from the artificial limiter may lead to deviations from the actual solution. Hence the need for a robust method capable of handling stochastic fluctuations properly. In this work we present a finite-volume numerical approximation for stochastic gradient flows with nonlinear energy functionals, based on a hybrid upwind-central discretisation of both the deterministic and stochastic fluxes.
This is a generalisation of a recently proposed finite-volume method for nonlinear nonlocal equations with a gradient flow structure [4]. The positivity of the density is ensured by an innovative time-adapting procedure based on the concept of Brownian trees. Both implicit and explicit temporal integrators are implemented. We exemplify the applicability and versatility of our method by solving the FH in a wide spectrum of physical settings included homogeneous nucleation of Lennard-Jones systems.

Selected references:


3:00pm - 3:30pm

Droplet coalescence commences in a ‘thermal regime’

Sreehari Perumanath, Matthew K. Borg, Mykyta V. Chubynsky, James E. Sprittles, Jason M. Reese

University of Edinburgh, Edinburgh, United Kingdom; University of Warwick, Coventry, United Kingdom

Starting from understanding how a storm cloud forms in the atmosphere to improving the quality of the printers in our offices, droplet-based systems are ubiquitous in our day-to-day life. Many times, such systems involve two or more droplets coalescing to become a larger one, and until now we only had a limited understanding of what was going on when two droplets touch each other for the first time. The classical notion of the coalescence of two droplets is that surface tension drives an initially singular flow. In this work we show, using molecular dynamics, that coalescence commences in a thermal regime in which single or multiple bridges form due to the presence of thermal capillary waves. The bridges expand linearly in time much faster than the viscous-capillary speed due to collective molecular jumps near the bridge fronts. Transition to the classical hydrodynamic regime only occurs once the bridge radius exceeds a thermal length scale and so this requires to be considered in hydrodynamic analyses of droplet coalescence.

1:30pm - 3:30pm

Minisymposium 16A: Toy mathematical models in the physical sciences

Session Chair: Philippe Trinh

1:30pm - 2:00pm

A toy model of exponentially-small instabilities in geophysical flows

Stephen David Griffiths

University of Leeds, United Kingdom

The linear stability of rotating shear flows is crucial to understanding various phenomena in atmospheric and oceanic fluid dynamics. Most such instability problems yield an instability that onset sets as some control parameter p (perhaps a wavenumber or shear strength) passes through a critical value p_c, with the growth rate then increasing as some positive power of p - p_c. However, here we investigate an apparently simple instability problem in which the growth rate is exponentially small as p passes through p_c.

This remarkable instability emerges in the context of equatorial fluid dynamics. The relevant toy model involves an idealisation of the Earth’s spherical geometry as a planar geometry (the equatorial beta-plane), along with the simplest possible assumptions about the density stratification (uniform) and disturbance structure (sinusoidal in longitude and height). The governing linear shallow-water equations can then be reduced to a well-known eigenvalue problem for the disturbance frequency (or growth rate), involving a rather complicated second-order ODE in latitude. With no background flow, this leads to various types of equatorial wave, which propagate along the equator but are trapped in latitude (with exponentially decaying tails). However, when the simplest possible non-trivial flow is added (with uniform latitudinal shear), one of the equatorial waves — the Kelvin wave — becomes unstable, with the growth rate being exponentially small in the limit of vanishing shear. This result has been established numerically by Natarov and Boyd, who also speculated as to the underlying mathematical cause.

Here we show how the growth rate and full spatial structure of the Kelvin-wave instability may be derived using matched asymptotics applied to the toy model (i.e., the shallow-water equations on the equatorial beta-plane). This involves an adventure with Whittaker functions in the exponentially decaying tails of the Kelvin waves, and a trick to reveal the exponentially small growth rate from a formulation that only uses regular perturbation expansions. Numerical verification of the analysis is also interesting and challenging: it turns out that the growth rate scales as p^3 \exp(-1/p^2) in the limit of small shear p, meaning that special high-precision calculations are required even when p is not that small (e.g., 0.2).

2:00pm - 2:30pm

A toy model of coastal outflows

Sean Jamshidi, Edward Johnson

University College, London, United Kingdom

The flow of river water into the sea transports nutrients, pollutants and sediment from the land to the ocean, and as such the dynamics of coastal outflow plumes is an important area of study. Laboratory experiments and numerical models of outflows reveal two distinct features: a coastal current that propagates rightward in the Northern hemisphere due to Coriolis, and a growing ‘buige’ that traps some of the outflow near the river mouth. The dynamics within the bulge are strongly nonlinear, with several factors influencing the bulge shape and the fraction of the outflow that it traps. This talk develops a toy model that isolates the effect of source.
vorticity. Briefly, regions of the outflow with cyclonic vorticity tend to propagate rightwards due to the image effect, reinforcing the coastal current, while regions with anticyclonic vorticity initially propagate leftwards and feed the bulge. We explore this phenomenon using a simple quasi-geostrophic model that allows the vorticity profile of the outflow to be completely specified, and derive analytical solutions that show that bulge formation need not occur if the outflow is dominated by cycloic vorticity.

2:30pm - 3:00pm
A toy model for flows through vegetation

Clint Y. H. Wong¹, Philippe H. Trinh², S. Jonathan Chapman¹

¹University of Oxford, United Kingdom; ²University of Bath, United Kingdom

The study of fluid flows interacting with vegetative structures presents a significant theoretical and numerical challenge on account of its inherently multi-scale nature. Consider, for example, the case of fluid passing over a submerged vegetative bed or layer. Even in the case of inelastic vegetation, the flow characteristics can be highly dependent on the configuration of the bed. In this talk, we will analyse this fluid-structure problem using relatively compact models, which now incorporates elastic deformation of the vegetation. A stability analysis of this problem suggests that shear at the top of the canopy is a dominant factor in determining the relevant threshold for flow instability. Furthermore, plant deflection encourages the temporal growth of perturbations, which resembles Kelvin-Helmholtz instability on mixing layers.

3:00pm - 3:30pm
A toy model for aeroacoustic catastrophes

Christopher John Howls, Jon Stone, Rodney Self

University of Southampton, United Kingdom

Recent work on high-frequency flow-interaction effects for 3D jet engine noise in a moving media uncovered unusual and previously unseen upstream beaming of significant amounts of acoustic energy, with implications for statutory noise measurements. These can be modelled by easily calculable, caustic structures of catastrophe theory. Significant "fang-like" features were also identified in the sound field that needed explaining since they have potentially serious engineering implications, but which appeared to violate mathematical aspects of both classical ray and catastrophe theories. A toy model was derived, involving complex rays that, a posteriori, resolved these problems and provided a comprehensive explanation, making links between the aeroacoustic problem, black hole event horizons and the Severn Bore.

1:30pm - 3:30pm
Minisymposium 7: Nonsmooth Dynamical Systems: From Nodes to Networks.

Session Chair: Yi Ming Lai

1:30pm - 2:00pm
Analysis of networks where discontinuities and nonsmooth dynamics collide: understanding synchrony

Yi Ming Lai

University of Nottingham, United Kingdom

The study of coupled oscillator networks in biology, physics and engineering is now commonplace. One powerful method for studying synchrony in such networks is the master stability function (MSF), which reduces much of the problem to analysis of a low-dimensional variational equation around a periodic orbit. This can be augmented by using a piecewise linear (PWL) modelling approach, which makes the orbits accessible in closed form. However, care must be taken when the nodes in the network have jump interactions, such as pulsatile synapses or impact in physical systems. When these occur at the same time as discontinuities in the underlying orbit, they may lead to an ordering problem which has no counterpart in smoothly coupled limit cycle systems. Moreover, the smoothed versions of jump interactions do not capture the behaviour of the nonsmooth model. Here we demonstrate this in a network of integrate-and-fire neurons as well as a network of Wilson-Cowan populations.

2:00pm - 2:30pm
Asynchronous networks of phase oscillators with dead zones

Christian Bick

University of Exeter, United Kingdom

Asynchronous networks provide a framework to understand networked systems with time and state-dependent network structure. Here, we discuss a particular class of asynchronous networks where the nodes are phase oscillators and state-dependent interactions are induced by "dead zones" (regions without interaction) in the coupling function and analyze the dynamics. Such interactions are relevant for networks where units have a refractory period where they are insensitive to new input. (This is joint work with P. Ashwin, M. Field, C. Poignard.)

2:30pm - 3:00pm
Dynamics in the switching layer -- mysteries and methods

Mike Jeffrey

University of Bristol, United Kingdom

A lot has been achieved in recent decades in extending traditional concepts of dynamical systems (like equilibria, bifurcations, and stability analysis) to nonsmooth systems. The missing ingredient has always been a sufficiently general and yet explicit way to handle the thing that puts the "non" in the "nonsmooth" -- the discontinuity itself. In recent years we have filled in this missing step. A 'discontinuity threshold' is blown up
into a 'switching layer'. Inside the layer we can carry out linearization and stability analysis just as for smooth systems, with a few novel multi-scale features. But where there is discontinuity there is indeterminacy -- we cannot escape the fact that a discontinuity brings into being many possible dynamical behaviours. We can distinguish between different outcomes by means of nonlinear terms inside the switching layer, bringing to life a whole new world of nonlinear dynamics "hidden" inside the discontinuity itself. Finally, these nonlinear terms bare an interesting relation to the divergent tails of asymptotic expansions about infinity (i.e. about points far from the discontinuity), giving us a rigorous interpretation of the sense in which "nonsmooth" models can be considered approximations.

3:00pm - 3:30pm
The nonsmooth dynamics of sleep-wake regulation
Anne C Skeldon
University of Surrey, United Kingdom

We are usually awake or asleep for hours at a time, but transition between wake and sleep on the timescale of seconds. Consequently, models of sleep-wake regulation typically exhibit behaviour on timescales separated by several orders of magnitude. In this talk I will give a brief overview of some current models of sleep-wake regulation and the associated dynamical structures.

I will show how models can be used to inform the policy debate on whether or not we should stop switching between standard time and daylight saving time and provide guidance on appropriate school start times for adolescents.

1:30pm - 3:30pm
Minisymposium 24: Machine Learning and Inverse Problems
Session Chair: Mohammad Golbabaee

1:30pm - 2:00pm
Computational MRI: from compressed sensing to machine learning
Mike Davies
University of Edinburgh, United Kingdom

Rapid MRI imaging has been one of the early beneficiaries of developments in compressed Sensing. This talk will discuss recent advances in rapid quantitative MRI based on the emerging protocol of Magnetic Resonance Fingerprinting (MRF). MRF can be considered as a generalized compressed sensing style inverse problem and exploits a particular data driven signal model derived from the MR physics. We will discuss the computational and algorithmic challenges of such techniques and also consider the role of machine learning can play in helping solve such inverse problems.

2:00pm - 2:30pm
Robustness and geometry of deep neural networks
Alhussein Fawzi
DeepMind, United Kingdom

Deep neural networks have recently shown impressive classification performance on a diverse set of visual benchmarks. When deployed in real-world environments, it is equally important that these classifiers satisfy robustness guarantees. In this talk, I will first highlight the vulnerability of state-of-the-art classifiers to simple perturbation regimes, such as adversarial and universal perturbations. Then, I will show the existence of fundamental connections between robustness and geometric properties of classifiers. In particular, I will show that the geometric analysis of the decision boundaries of deep neural networks provides key insights into their robustness. I will finally conclude with important open problems in this emerging field.

2:30pm - 3:00pm
Adversarial regularizers in inverse problems
Sebastian Lunz
University of Cambridge, United Kingdom

We discuss an approach to use neural networks as a regularisation functionals for inverse problems. The network is trained as a critic, telling apart clean images from those corrupted with typical noise. Once trained, it is used as a regularisation functional within a variational approach to inverse problems. We demonstrate results on computed tomography for lung scan data.

3:00pm - 3:30pm
Four dimensional ultrasound tomography with real data via traditional inversion and via machine learning
Manuch Soleimani
UoB, United Kingdom

Tomographic imaging is a highly multi-disciplinary field involving applied maths, computer science, engineering, medicine and more. In this talk we focus on our recent work in ultrasound tomography for crystalisation process. We present spatio-temporal imaging of a moving object(s) for ultrasound tomography in 2D and 3D. Additionally, we present an overview of other tomographic imaging studied in our lab. Engineering tomography lab (ETL) works in a wide range of inverse problems for different types of tomographic imaging for medical and industrial applications. Recent example is our collaboration with CERN on a join X-ray tomography GPU based software platform TIGRE, an update of the most recent development will be presented. Many applications in ETL involves nonlinear inverse problem, high dimensional
reconstruction, and multi-physical modelling of the real world applications. The use of statistical based methods as well as AI based approach will be also be presented.

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<th>1:30pm - 2:00pm</th>
<th>Minisymposium 14A: Mathematical Modelling of Lithium-Ion Batteries</th>
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| CB 3.6 | Session Chair: Matthew Hunt  
| | Session Chair: Jamie Michael Foster |
| | **Multiscale modelling of cylindrical lithium ion battery temperature profiles**  
| | Matthew Hunt, Ferran Brosa-Planella, Florian Theil, Dhammika Widanalage  
| | University of Warwick, United Kingdom  
| | There has been a great deal of work done on the multiscale continuum modelling of lithium ion batteries since the seminal paper on the topic by Newman with many simplifications and generalisations of it since. In this talk we will present a new model which is a formal homogenisation of the basic microscale equations which will include temperature as a key feature. The formal mesoscale electrochemical model will be derived and then the macroscale model for the temperature equation. Some asymptotics will be shown at the end for fast discharge of batteries. |

| 2:00pm - 2:30pm |
| | **Mathematical insights into heat generation in lithium-ion batteries**  
| | Matthew G. Hennessy¹, Iain R. Moyles²  
| | ¹University of Oxford, United Kingdom; ²York University, Canada  
| | Lithium-ion batteries (LIBs) are ubiquitous in modern society and are the primary energy source for portable electronic devices and electric cars. Despite the many attractive features of LIBs, several incidents involving overheating and exploding batteries have led to severe safety concerns. This has prompted the development of detailed thermo-electro-chemical models that can be used to predict the thermal response of an LIB. In this talk, we will show how such a model can be systematically reduced to a system of nonlinear ordinary differential equations which, under certain conditions, can be solved analytically. The reduction not only elucidates the dominant mechanisms of heat transport, but also gives new insight into how the capacity of a battery can be inferred from its instantaneous thermal response. Furthermore, the reduced thermal model is ideal for use in real-time battery management systems. |

| 2:30pm - 3:00pm | **Asymptotic Reduction of Battery Models**  
| | Scott Marquis  
| | University of Oxford, United Kingdom  
| | Full order continuum models are too complex to employ on the limited data available in real world applications of lithium-ion batteries such as electric buses, ferries, and planes. By using asymptotic methods, we systematically derive simplified models which are faster and easier to parameterise than the full continuum models but are still fundamentally based upon the underlying physics. We begin by introducing the standard one dimensional model of a lithium-ion battery, the Doyle-Fuller-Newman (DFN) model, and then identify key dimensionless parameters in this model. By making asymptotic expansions, we derive the commonly used Single Particle Model (SPM) at leading order. We then proceed to the next order to derive an extended SPM, which we compare with other attempts to extend the SPM in the literature. Finally, we conclude by presenting the extension of our results to three dimensions. |

| 3:00pm - 3:30pm | **The role of conductivity in facilitating fast (dis)charge in LFP electrodes**  
| | Jamie Michael Foster  
| | University of Portsmouth, United Kingdom  
| | Utilization of thicker electrodes is one route towards improving the energy density of Li-ion batteries because it decreases the number of electrodes per cell, thereby increasing the ratio of active material to current collectors. However, the increased thickness means that it is difficult to achieve sufficiently fast transport of the lithium to supply the deep regions of the electrode with reactant. At even moderate (dis)charge rates, thick electrodes exhibit significant polarization and undesirable under-utilization of capacity. We report experimentally determined lithium concentration profiles in a 300 micron thick graphite electrode under operation. The observed behavior clearly shows the phase transforms that are known to occur within graphite during (de)lithiation; there are sharp boundaries between graphite areas lithiated to different stages. Comparison with porous electrode theory modelling reveals that a portion of the Li is temporarily stored in the electrode surface film prior to intercalation. Although it is often difficult to fully lithiate the thick electrode, we demonstrate that the inclusion of a short current reversal, facilitates more complete lithiation. We also demonstrate the value of this high-fidelity experimental data to the modelling community, by showing how it can be used for high-confidence parameter estimation when combined with inverse modelling techniques. |

| 1:30pm - 3:30pm | **Contributed Talks 20: Waves 1**  
| | Session Chair: Ory Schnitzer |
| | 1:30pm - 1:50pm | **Slender-body theory for localized-surface-plasmon resonance**  
| | Matias Ruiz, Ory Schnitzer  
| | Imperial College, United Kingdom |
We propose a slender-body theory for calculating the surface-plasmon eigenvalues and eigenmodes of smooth high-aspect-ratio metallic nanoparticles (of otherwise arbitrary shape) and their resonant excitation by incident electromagnetic radiation. Analytical solutions to this problem are restricted to simple shapes, whereas slender bodies are commonly used in photonic devices. Using matched asymptotic expansions, we develop an equivalent one-dimensional model which is straightforward to solve numerically and in special cases furnishes closed form solutions.

1:50pm - 2:10pm

Wave manipulation on thin elastic plates

**Gregory James Chaplain**, Richard V. Craster

Imperial College London, United Kingdom

Structured thin elastic plates are capable of supporting array guided modes, which can be manipulated to produce a myriad of interesting effects for controlling wave propagation. In order to geometrically design such systems we introduce a spectral method, coupled with an asymptotic scheme, for efficiently calculating dispersion relations of structures which support waves characterised by periodic behaviour in one direction and exponential decay in the orthogonal direction. Such waves have recently received much attention in the world of topological wave mechanics, and we apply our methodology to these cases and present new uses of graded structures to produce rainbow trapping effects for the design of flat lenses. The analysis presented carries over to electromagnetic and acoustic settings, providing motivation for the design of new photonic and phononic devices.

2:10pm - 2:30pm

Effective transparency of dense metallic crystals

**Ory Schnitzer**, Richard V. Craster, Rodolfo Brandao

Imperial College London, United Kingdom

Electromagnetic waves cannot propagate in metal, instead they attenuate on a short length scale termed the "skin depth." For example, the skin depth for Aluminium at a vacuum wavelength of 200 microns is just 67 nanometers.

Nevertheless, it has been recently demonstrated numerically that crystals formed of doubly periodic arrays of metallic cylinders are effectively transparent to infrared TE- polarised radiation [S. Palmer et al., arxiv:1811.08796] — even when the cylinders are nearly touching. Thus, the real part of the effective index of refraction is positive and increases as (i) the spacing between the cylinders decreases and (ii) the skin depth of the metal increases (until it becomes comparable to the cylinder radius); the imaginary part of the effective index varies in a complicated way with these parameters, and with frequency, but remains surprisingly small. Such dense metallic crystals therefore effectively constitute high-index materials having large attenuation lengths (several times the vacuum wavelength and many times the apparent wavelength in the crystal).

To study the effective properties of such metallic crystals we adopt the method of "high-contrast homogenization," which corresponds to taking the long-wavelength limit while properly accounting for the huge complex values of the metal's dielectric function. Thus the macroscale field satisfies an effective wave equation in which the permittivity tensor is governed by an external "cell problem" (which is identical to that found in classical homogenisation for perfectly conducting cylinders) and a scalar permeability governed by an internal cell problem. We explain the singularity of the index in the densely packed limit, and the dependence on skin depth, by analysing the external and internal cell problems, respectively, using the method of matched asymptotic expansions. We thereby obtain closed-form expressions for the complex-valued effective-index tensor for nearly arbitrary inclusion and lattice geometries. These analytical results are virtually indistinguishable from the finite-element computations in Palmer et al..

2:30pm - 2:50pm

Extraordinary transmission through a narrow slit

**Jacob R. Holley**, Ory Schnitzer

Imperial College London, United Kingdom

We revisit the problem of extraordinary transmission of acoustic (electromagnetic) waves through a slit in a rigid (perfectly conducting) wall. We use matched asymptotic expansions to study the pertinent limit where the slit width is small compared to the wall thickness, the latter being commensurate with the wavelength. Our analysis focuses on near-resonance frequencies, furnishing elementary formulae for the field enhancement, transmission efficiency, and deviations of the resonances from the Fabry–Perot frequencies of the slit. We find that the apertures' near fields play a dominant role, in contrast with the prevalent approximate theory of Takakura [Physical Review Letters, 86 5601 (2001)]. Our theory agrees remarkably well with numerical solutions and electromagnetic experiments [Suckling et al., Physical Review Letters, 92 147401 (2004)], thus providing a paradigm for analyzing a wide range of wave propagation problems involving small holes and slits.

2:50pm - 3:10pm

Acoustic scattering from bubbles trapped in micro-grooves

**Rodolfo Brandao**1, Ehud Yariv2, Ory Schnitzer1

1Imperial College London, United Kingdom; 2Technion — Israel Institute of Technology

Acoustic metamaterials formed by locally resonant structures posses remarkable capabilities of enhancing, focusing and guiding the propagation of sound waves. Micro-bubbles are often employed as the locally
In this talk, we suggest to consider so-called "superhydrophobic surfaces" as natural candidates for realising highly tuneable, bubble-based acoustic metasurfaces. We focus our attention on a canonical superhydrophobic configuration formed of a solid substrate decorated with a periodic array of micro-grooves; it is assumed that each groove traps an air bubble whose meniscus is pinned to the groove's corners. While such superhydrophobic surfaces have been widely explored in the context of wetting and drag reduction, their acoustic properties have not been previously investigated.

We begin by discussing the scattering by a single trapped bubble. We exploit the smallness of the gas-liquid density ratio and employ matched asymptotic expansions to obtain the complex amplitude of the emitted cylindrical wave, as well as a reduced description of the meniscus oscillation and the near-field pressure fields. Due to the combination of compressibility, surface tension, and pinning effects, the acoustic response of the trapped bubble exhibits a rich frequency response, which includes a fundamental resonance followed by a sequence of closely spaced resonance and anti-resonance pairs.

Building on the above theory for a single bubble, we proceed to investigate arrays of trapped bubbles. By employing Foldy's point-scatterer approximation, we find that, for infinite arrays, strong inter-bubble interactions shift, and diminish the amplitude of, the resonance peaks. The frequency response of long-finite arrays exhibits highly oscillatory deviations from that of an infinite array in a sequence of shrinking frequency intervals. These deviations are shown to be associated with edge-excitation of surface "spoof-plasmon" waves.

3:10pm - 3:30pm
Friedlander-Keller Ray Expansions and Scattering at Perturbed Boundaries
Anthony Marko Rade Radjen
University of Nottingham, United Kingdom
AMR Radjen, RH Tew, and G Gradoni

The standard ray approach to solving the Helmholtz equation in the large wavenumber limit involves seeking solutions having an oscillatory exponential, with phase linear in that wavenumber, multiplying an amplitude expansion expressed in terms of inverse powers of it. The Friedlander-Keller modification to this procedure incorporates an extra power of the wavenumber (in addition to the linear one) within the phase of the pre-exponential to the amplitude expansion, with this extra term being essential in certain types of high-frequency diffracted wave.

Examples involving wave scattering from a class of perturbed boundaries in acoustics, electromagnetism and elasticity demonstrate that sometimes more such phase terms, and a consequent extension to the Friedlander-Keller methodology, are needed and we present (by way of examples) an outline theory for this eventuality.

1:30pm - 3:30pm
Session Chair: Dietmar Hoemberg
Session Chair: Katerina Kaouri

1:30pm - 2:00pm
MI-Net networking lunch continues

2:00pm - 2:25pm
Science Shops and European Study Groups with Industry: European synergies for tackling societal challenges in the open science era
Katerina Kaouri1,2

1School of Mathematics, Cardiff University, United Kingdom; 2SciCo Cyprus, Cyprus

For an industrial mathematician the word "industry" stands for any activity of societal and/or economic value and a plethora of important societal challenges have been tackled in the European Study Groups with industry (ESGIs) and in other projects. ESGIs are week-long academia-industry workshops coordinated by the European Consortium of Mathematics in Industry since the 80s, after originating in Oxford in 1968. Many ESGIs have been recently funded by the EU COST Action “Mathematics for Industry Network” (MI-NET), including ESGI125 and ESGI146 that I coordinated in Cyprus in 2016 and 2018, leading to many successful academia-industry collaborations.

On the other hand, 10 new Science Shops have been recently launched in Europe, through the EU project SciShops.eu. Science Shops are entities which undertake or facilitate research on pressing societal challenges, in collaboration with civil society. Science Shops and the industrial mathematics community are both operating within the “open science” realm and it is obvious that they have common objectives. In ESGI146, which was co-funded by SciShops.eu, and was also a “co-creation event with society” we brought together these two communities and worked on pressing societal challenges such as the gender pay gap and fuel consumption.

In this talk I will present societal challenges tackled in ESGI146 and in other ESGIs and will invite brainstorming and discussions on how the industrial mathematics community can further collaborate with Science Shops and other open science initiatives in Europe.

2:25pm - 2:50pm
Physically feasible decomposition of Engino® toy models: A graph-theoretic approach

Miguel David Bustamante¹, Efstathios Antoniou², Adérito Araújo³, Avir Gibali⁴

¹University College Dublin, Ireland; ²Alexander Technological Educational Institute of Thessaloniki, Greece; ³University of Coimbra, Portugal; ⁴ORT Braude College, Israel

During the 125th European Study Group with Industry held in Limassol, Cyprus, 5-9 December 2016, one of the participating companies, Engino.net Ltd, posed a very interesting challenge to the members of the study group. Engino.net Ltd is a Cypriot company, founded in 2004, that produces a series of toy sets -- the Engino® toy sets -- consisting of a number of building blocks which can be assembled by pupils to compose toy models. Depending on the contents of a particular toy set, the company has developed a number of models that can be built utilising the blocks present in the set. However, the production of a step-by-step assembly manual for each model could only be done manually. The goal of the challenge posed by the company was to implement a procedure to automatically generate the assembly instructions for a given toy. In the present paper, we propose a graph-theoretic approach to model the problem and provide a series of results to solve it by employing modified versions of well established algorithms in graph theory. An algorithmic procedure to obtain a hierarchical, physically feasible decomposition of a given toy model, from which the assembly instructions can be recovered, is proposed.

2:50pm - 3:15pm
ESG 137: Total Hip Arthroplasty Workshop Report

Jacqueline Christmas¹, Ana Avdzhieva², Blanca Lichtblau³, Jiafeng Xu⁴, Markus Grasmair⁵, Torbjorn Ringholm⁶, Heinrich Bruggemann⁷

¹University of Exeter, United Kingdom; ²Sofia University "St. Kliment Ohridski"; ³NTNU; ⁴Technische Universität Berlin; ⁵Helse Stavanger; ⁶Stavanger Universitetssjukehus

In most OECD countries, the number of hip replacement operations performed has increased rapidly since 2000 and is considered as the most effective intervention for severe osteoarthritis and hip fractures. In Sweden alone, over 17000 hip surgeries were performed in 2016. Total hip arthroplasty (THA) has long been used to relieve pain, improve function, and to anatomically restore normal biomechanics for patients with severe hip joint diseases.

Before a THA operation takes place, the surgeon must plan the surgery and estimate the sizes of the replacement hip components to suit the patient. In order to support planning, a standardised X-ray is taken of the pelvic area and the upper parts of the femurs. In this workshop we investigated mathematical and computational means for automatically deriving shapes and measurements from the X-ray images, and report the results here.

Minisymposium 21A: Networks, Collective Behaviour and their Applications

Session Chair: Chris Antonopoulos

3:30pm - 5:00pm
CB 3.5

3:30pm - 4:00pm
Small-worldness favours network inference

Rodrigo A. Garcia, Arturo C. Marti, Cecilia Cabeza, Nicolás Rubido

Universidad de la República, Instituto de Física de Facultad de Ciencias, Iguá 4225, Montevideo, Uruguay

A main goal in the analysis of a complex system is to infer its underlying network structure from time-series observations of its behaviour. The inference process is often done by using bi-variate similarity measures, such as the cross-correlation (CC), however, the main factors favouring or hindering its success are still puzzling. Here, we use synthetic neuron models in order to reveal the main topological properties that frustrate or facilitate inferring the underlying network from CC measurements. Specifically, we use pulse-coupled Izhikevich neurons connected as in the Caenorhabditis Elegans neural networks as well as in networks with similar randomness and small-worldness. We analyse the effectiveness and robustness of the inference process under different observations and collective dynamics, contrasting the results obtained from using membrane potentials and inter-spike interval time-series. We find that overall, small-worldness favours network inference and degree heterogeneity hinders it. In particular, success rates in C. Elegans networks - that combine small-world properties with degree heterogeneity -- are closer to success rates in Erdős-Rényi network models rather than those in Watts-Strogatz network models. These results are relevant to understand better the relationship between topological properties and function in different neural networks.

4:00pm - 4:30pm
Topological Melting in Networks of Granular Materials

Najlaa Sadeq Alalwan

Strathclyde University, United Kingdom

We study the robustness of the network based on the percolation approach. We developed a new measure to find the critical threshold for edge failure by attack process, which indicates when the network is fragmented. This measure depends on the communicability between the nodes. More, as a result of that the granular materials represent a vast category of particle conglomerates with many areas of industrial applications. We represent these materials by graphs which capture their topological organization and ordering. Then, we use the communicability function to prove the existence of a universal topological melting phase transition in these graphs. This transition resembles the melting process occurring in solids. We show that crystalline-like granular materials melts at lower temperatures and display a sharper transition between solid to liquid phases than the random spatial graphs, which represent amorphous granular materials. In addition, we show the evolution mechanism of melting in these granular materials. In the particular case of crystalline materials the process starts by melting a central core of the crystal which then growth until the whole material is in the liquid phase.
Scaled consensus of switched multi-agent systems

Yilun Shang
Northumbria University, United Kingdom

In the past decades, distributed control of networked multi-agent systems has received a great deal of attention in the system and control community due to its broad applications in areas such as formation control, cooperative coordination of unmanned aerial vehicles, robotic teams and sensor networks. In this talk, we discuss the scaled consensus problem for switched multi-agent systems composed of continuous-time and discrete-time subsystems. By using the nearest neighbor-interaction rules, four types of scaled consensus protocols are presented to achieve, respectively, asymptotic, finite-time, fixed-time convergence rates, and resilient consensus. Based upon algebraic graph theory and Lyapunov theory, scaled consensus is shown to be reached for strongly connected networks. We explicitly express the final consensus states as some initial-condition-dependent values. Simulation examples are provided to illustrate the availability of theoretical results.

Minisymposium 19A: Different Viewpoints on Multi-Scale Problems

3:30pm - 5:00pm
CB 4.1

Session Chair: Hong Duong
Session Chair: Johannes Zimmer

String method for generalised gradient flows: computation of rare events in reversible stochastic processes

Tobias Grafke
University of Warwick, United Kingdom

Rare transitions in metastable stochastic processes can often be rigorously described via an underlying large deviation principle. Recent breakthroughs in the classification of reversible stochastic processes as gradient flows have led to a connection of large deviation principles to a generalized gradient structure. Here, we show that, as a consequence, metastable transitions in these reversible processes can be interpreted as heteroclinic orbits of the generalized gradient flow. This in turn suggests a numerical algorithm to compute the transition trajectories in configuration space efficiently, based on the string method traditionally restricted only to gradient diffusions.

Edge multiscale methods for elliptic problems with heterogeneous coefficients

Guanglian Li
Imperial College London, United Kingdom

In this talk, I will present two new types of edge multiscale methods to solve Partial Differential Equations (PDEs) with high-contrast heterogeneous coefficients: Edge Spectral Multiscale Finite Element Method (ESMsFEM) and Wavelet-based Edge Multiscale Finite Element Method (WEMsFEM). Their convergence rates for elliptic problems with high-contrast heterogeneous coefficients are demonstrated in terms of the coarse mesh size H, the number of spectral basis functions and the level of the wavelet space, which are verified by extensive numerical tests. This is a joint work with Shubin Fu and Eric Chung from Chinese University of Hong Kong.

Novel approaches for upscaling linear advection diffusion reaction processes in porous media

Matteo Icardi
University of Nottingham, United Kingdom

Although the macroscopic limit of linear advection-diffusion equations has been well understood since the early developments of porous media transport theory (through, for example, homogenisation, and volume averaging), its extension to complex flow regimes is still an open question, even in presence of well-separated spatial scales. This is due to the presence of non-trivial microscopic equilibrium configurations (compared to the trivial constant leading order solution obtained by standard periodic homogenisation), or of dynamic equilibrium configurations. For example, when dealing with fast surface reactions, high microscopic gradients can develop locally. Similarly, a conservative solute in the neighbourhood of a concentration source (injection) undergoes a dynamic evolution of the local microscopic configuration in time and space before reaching the asymptotic self-similar profile. These are only two examples where the classical upscaling approaches fail, and effective macroscopic equations are often found either empirically or by resorting to generic random walk models.

In this talk, we present some (old and) new theoretical frameworks to overcome these limitations without the need of an ad-hoc calibration or stochastic particle models. These generally involve solving more auxiliary local problems, and often computing local spectral properties (eigenvalues and eigenfunctions) of the underlying transport operators. In particular, we will focus on model-order reduction approach based on projections from the full multiscale formulation onto low-dimensional spaces, borrowing concepts from the finite element community (such as Hi-Mod, MsFEM, and VMM), and from statistical mechanics. New macroscopic equations are obtained for one or more macroscopic quantities, that can be seen as extended homogenised formulations. Applications of these techniques to the classical 2D Taylor dispersion in a channel and other heterogeneous periodic flows will be discussed.
Minisymposium 20A: Understanding the dynamics of particle and droplet impacts

3:30pm - 4:00pm

Skimming impacts and rebounds of arbitrarily shaped bodies on shallow liquid layers

Ryan Palmer, Frank Smith
UCL, United Kingdom

Investigated in this paper is the coupled body-fluid motion for a solid body (of arbitrary polygonic shape with zero thickness at the trailing edge) undergoing a skimming impact on a shallow water layer. The body shape is parametrized according to a curvature parameter $C$, for which the rebound dynamics of the motion are predicted. Both analysis of small-time water entry and water exit solutions are produced and are shown to be of close agreement with the numerical predictions. In modelling bodies of arbitrary shape there are two geometrical scenarios of interest: the concave case ($C < 0$ producing a hooked body) and the convex case ($C > 0$ producing a rounded underside). Reduced analysis and physical insights are made in each case alongside numerical investigations.

4:00pm - 4:30pm

High speed drop impact at arbitrary angles of incidence: a multi-scale approach to defining water collection efficiency

Radu Cimpeanu1, Demetrios Papageorgiou2
1University of Oxford, United Kingdom; 2Imperial College London, United Kingdom

The rich structures arising from the impingement dynamics of water drops onto solid substrates at high velocities will be discussed over a range of length- and timescales. Current methodologies in the aircraft industry for estimating water collection are based on particle trajectory calculations and extensions thereof in order to approximate the complex fluid-structure interactions. The presented approach incorporates the detailed fluid dynamical processes often ignored in this setting, such as the drop interaction with the surrounding air flow, drop deformation, rupture and coalescence, as well as the motion of the ejected microdrops in the system. One-to-one comparisons are performed with experimental data available in the pre-impact stage, while the early stages of the impact itself are validated using an extension of the asymptotic analysis machinery provided by Wagner theory. The main body of results is created using parameters relevant to flight conditions with droplet sizes in the range of tens to several hundreds of microns impacting at speeds of up to 100 m/s.

4:30pm - 5:00pm

The impact of wrinkling on impact

Doireann O'Kiely1, Finn Box1,2, Ousmane Kodio1, Maxime Inizan1, Alfonso Castrejon-Pita1, Jonathan Whiteley1, Dominic Vella1
1University of Oxford, United Kingdom; 2Manchester Centre for Nonlinear Dynamics, University of Manchester

Impact at a liquid-air interface is altered when a thin elastic sheet floats on the liquid surface. A ripple propagates out from the point of impact, but has a waveform $\sim t^{1/2}$ rather than the $\sim t^{1/3}$ typical of capillary waves. However, this square root behaviour also deviates from the classical Wagner result.

In this talk we demonstrate that the behaviour of the `elastocapillary ripple` arises due to the formation of wrinkles in the floating elastic sheet. We reduce this new impact problem to a one-parameter similarity problem, which interpolates between the limits of a point impactor and Wagner theory. We also explore the evolution of the wrinkle pattern in the elastic sheet.

Minisymposium 22A: Inverse Problems: Theory and Applications

3:30pm - 5:00pm

Variational networks: learning regularisation operators for inverse problems

Martin Benning1, Erich Kolber2, Thomas Pock3
1Queen Mary University of London, United Kingdom; 2Graz University of Technology, Austria

We discuss so-called variational networks and their use as learned regularisation methods for ill-posed inverse problems. We present different network architectures, discuss the training of the network’s model parameters and show corresponding numerical results. We conclude with theoretical results concerning the stability of those networks as well as convergence behaviour.

4:00pm - 4:30pm

Influence of numerical discretisation on object characterisation in inverse problems

Alan A. S. Amad1, Paul D. Ledger1, William R.B. Lionheart2
1Swansea University, United Kingdom; 2The University of Manchester, United Kingdom

In this talk we are interested in characterising small conducting permeable objects to aid with the solution of electromagnetic inverse problems. Imaging modalities include metal detection, electrical impedance...
tomography (EIT), magnetic impedance tomography and ground penetrating radar while applications range from security screening to identifying landmine and medical imaging to name but a few.

For a range of different problems, asymptotic formulae have been derived for the perturbed electromagnetic field caused by presence of small object as the size of the inclusion goes to zero. In each case, the object has been found to be characterised by a rank 2 polarizability tensor. This rank 2 tensor contains information about the shape and material properties of the object and is independent of its position.

The form of the tensor varies depend on the frequency of the imaging modality, but takes its simplest form in electrical impedance tomography. In this case it coincides with the Polya-Szego tensor. The Polya-Szego tensor is also known to have other important practical applications in hydrodynamics, electrostatics, and in elasticity composite material problems.

In order to compute the Polya-Szego tensor for different shaped objects, it is necessary to solve a scalar transmission problem with appropriate jump conditions. The tensor coefficients are then obtained by post-processing integrals of the solutions to such problems. It is known to be symmetric and analytical formulae are available for simple objects such ellipsoids and disks. For other objects a numerical procedure must be used.

A variety of different numerical methods can be used for the approximate computation of the tensors coefficients including the finite element method and boundary integral approaches. However, numerical experiments have shown that the resulting tensors are not always symmetric, particularly when discretised layer potentials are used. This can cause problems when computing its eigenvalue decomposition to aid with object identification.

This talk will investigate the relationship between computational discretisation, accuracy and symmetry of the computed tensor coefficients for a range of object shapes.

4:30pm - 5:00pm
A computationally efficient regularisation strategy for Ensemble Kalman Inversion
Yuchen Yang, Marco Iglesias
University of Nottingham, United Kingdom

Recent work has shown that Ensemble Kalman Inversion (EKI) algorithms can be successfully used as derivative free solvers for PDE-constrained identification problems. EKI can be derived by using ensemble covariances to approximate Frechet derivatives in the update formulas for the regularising Levenberg-Marquardt (LM) scheme. The accuracy and stability of EKI thus relies on the selection of a regularisation parameter that appears in the Kalman update formula within EKI. Numerical evidence has shown that importing parameter selection rules from the LM technique can provide stability to EKI for sufficiently large ensemble size. However, in some cases, such a selection of regularisation parameter can lead to very slow convergence of the EKI algorithm. This is particularly the case for problems where the underlying unknown is discontinuous and where the regions of discontinuity display geometric features with variable length scales (that must be inferred from the data). In this talk we introduce a new approach for the selection regularisation parameter which involves the data misfit only and that can improve the efficiency of EKI in at least 50%. We motivate this rule from a Bayesian interpretation of EKI and we provide numerical examples from in inverse problems with various applications in science and engineering.

3:30pm - 5:00pm
Minisymposium 23B: The Mathematics for Industry Network Mi-Net – a European success story

CB 1.11
Session Chair: Dietmar Hoemberg
Session Chair: Katerina Kaouri

3:30pm - 3:45pm
Coffee break

3:45pm - 4:10pm
Elkem and Industrial-focused mathematicians – More than 30 years of fruitful collaboration
Aasgeir Valderhaug
Elkem ASA, Norway

Elkem ASA is a global manufacturer of silicon alloys and silicone materials with headquarter in Norway. Elkem has regularly given problems at The Mathematical Study Group with Industry since the mid 80’s and has attended to around 20 study groups. This has given Elkem a professional network within industrially applied mathematics, and because of this, Elkem was invited to be an industrial member of the Industrially Focused Mathematical Modelling - Centre for Doctoral Training at University of Oxford from 2015. Elkem has five DPhil students at Oxford and more than ten internships have been working at Elkem R&D Centre in Kristiansand.

Elkem is an industrial manufacturing company with a relatively large R&D organisation, but mainly on material science and engineering. The “density of mathematicians” is very low, so what are the reasons for Elkem’s strong involvement within this area?

Several of Elkem’s main production processes have the following characteristics:
- Limited knowledge about the actual process reactions and mechanisms.
- Lumped production processes with a complex pattern of inter-connected sub-processes.
- Very high process temperatures (T > 2000°C). Few direct measurements of internal process variables.
- The operation often based on output variables and manual observations.
- Manual control of important process conditions.

Modelling, and especially PDE modelling with nondimensionalisation, has shown to be a powerful tool to increase the “process understanding” of Elkem’s processes.

Elkem’s objectives are to increase the efficiency in today’s silicon alloy production and develop novel processes to meet the “zero emission” requirements of 2050. Thus, there is an increased need for detailed process understanding to improve process design and developing more efficient production technology. Applied mathematics will be an important tool for Elkem in this work.

4:10pm - 4:35pm

Imaging nanoparticles with visible light: an Industrial Mathematics case study
Tim Myers, Wolfgang Bacsa
Centre de Recerca Matematica, Spain; CEMES, Toulouse

It is well-known that the wavelength of visible light (between 400-700nm) is too large to observe nanoparticles. Hence the observation of single nanoparticles typically requires the use of transmission or scanning electron microscopy. This equipment is expensive and requires a vacuum or low pressure environment which often affects the particle’s properties and changes its structure. It is therefore desirable to be able to use a less invasive optical method within an ambient atmosphere.

Experimental scientists in the Centre d’Elaboration de Materiaux et d’Etudes Structurales in Toulouse have developed a method to record the diffraction pattern created by the interference between a laser and the light emitted by a nanoparticle subjected to this beam using a pointed optical fibre. During a two month MI-Net Short Term Scientific Mission to Toulouse we derived a mathematical model to recreate the diffraction pattern. It was then shown that with only two simple measurements we were able to locate the particle. Thus we developed a fast and cheap method to find nanoparticles using visible light. The mathematical solution also predicts the phase shift of the scattered wave, a quantity that is notoriously difficult to measure, however this is very sensitive to errors.

4:35pm - 5:00pm

Neural Networks and Arbitrage in the VIX – A Deep Learning Approach for the VIX
Joerg Robert Osterrieder
ZHAW, Switzerland

The Chicago Board Options Exchange (CBOE) Volatility Index, often referred to as VIX Volatility Index (VIX), is considered by many market participants as a common measure of market risk and investors’ sentiment. It is also sometimes called the fear index. In general, the VIX represents the market's expectation of the 30-day-ahead looking implied volatility obtained from real-time prices of options on the S&P 500 index.

Over the last few years, many claims about possible VIX manipulations have been brought up by market participants. The increased attention on the VIX has been revived again by unusual trading patterns, which were observed on the market, on February 5 and April 18, 2018.

While smaller deviations between implied and realized volatility are a well-known stylized fact of financial markets, large, time-varying differences are also frequently observed throughout the day. In theory, such large deviations might lead to arbitrage opportunities on the VIX market. However, it is hard to exploit as the potential replication strategy requires buying several hundred out-of-the-money (put and call) options on the S&P 500 index. In addition, the potential list of options used for building the replication strategy constantly changes due to underlying price movements, making it difficult to implement it in real-time. Finally, in most cases, the theoretical replication strategy involves high transaction costs which are driven by illiquid options.

This paper discusses a novel approach to replicating and predicting the VIX by using just a subset of the most liquid options. The presented approach is based on a recurrent neural network, more precisely on a long short-term model (LSTM) and it uses intraday data of S&P 500 options and the VIX. The results can be used to find a much more cost-efficient way of replicating the VIX and exploiting any arbitrage opportunities.

To the best of the authors’ knowledge, this is the first paper, that describes a new methodology on how to replicate the VIX (to potentially exploit arbitrage opportunities using VIX futures) and applies most recently developed machine learning models to intraday data of S&P 500 options and the VIX. The presented results are supposed to shed more light on the ongoing discussions about possible market manipulations, help other investors to better understand the market and support regulators to investigate market inefficiencies.

4:00pm - 5:00pm

Minisymposium 17A: Non-convex methods in inverse problems
Session Chair: Sean Fraser Holman

4:00pm - 4:30pm

Weakly-convex Multibang Regularization in Passive Radiation Imaging
Philip, John Richardson, Sean Holman
University of Manchester, United Kingdom

Applications for accurate reconstructions from Passive Radiation Imaging are widespread from medical imaging to security. Unfortunately reconstructing such images is often an ill-posed problem and require regularization. One recently developed regularizer known as Multibang makes use of a priori information about the possible attenuation values in an object to both improve reconstructions and reduce the amount of measured data required. The original version of Multibang is a convex penalty term allowing use of the rich world of convex optimisation. We instead discuss the motivation for the inclusion of a weakly convex penalty, as well as using theoretic results to show how we can apply a variant of Alternating Direction Method of Multipliers(ADMM), even in this non-convex setting. We conclude by showing numerical results obtained by such a method and discuss further research avenues.
How do individuals' personality traits influence the community survival?

**Martina Testori¹, Hedwig Eisenbarth², Rebecca B. Hoyle¹**

¹School of Mathematical Sciences, University of Southampton, United Kingdom; ²School of Psychology, Victoria University of Wellington, New Zealand

Mathematically modeling how humans make decisions has become one of the most interesting challenges that the academic world has tackled in the last fifty years.

A focal point of these models is that humans are not purely rational as initially postulated, but are influenced by a wide range of factors, both endogenous (e.g. personality traits, current mood) and exogenous (e.g. society, cultural environment). Using evolutionary game theory and numerical simulations, we investigate how psychopathic personality traits affect both group dynamics and community evolution. Our goal is to provide insight into the circumstances under which the existence of high values of psychopathic traits in some members of the community is advantageous for the population as a whole.

In our work, we investigate how specific aspects of psychopathic traits influence decisions both at the individual and at the group level. Psychopathy is usually described as a constellation of personality traits which include lack of guilt and fear, impulsivity, emotional detachment, impairment in building strong relationships, dishonesty and callousness. As such, psychopathic traits are usually associated with behaviours of negative valence, but this is not always in lines with those personality traits persisting in society.

Through individual-based models, we reproduced the evolution of a community composed of both high and low psychopathic individuals in different environmental conditions. Simulating both benevolent and harsh environments, we observed that high psychopathic community members can help society to overcome the period of crisis, thanks to their fearless attitudes.

In this sense, the presence of high psychopathic individuals in a community can be determinant for its survival.

Our research provides a mathematical framework linking psychopathic traits to the dynamics of community resources and survival, broadening the literature that focuses mainly on the impact of psychopathy on individuals. Based on our results, we claim that particular aspects of psychopathy present, to different degrees, in the general population (such as fearless behaviours, callousness, and boldness) can be beneficial in harmful situations, providing an advantage for survival.
Individual memory greatly influences how the individual and collective behaviour of a population evolve. In this talk, we consider a large well-mixed population of individuals faced by a general binary-choice problem, boiling down to picking one of two possible strategies. This applies to an array of social situations where interactions can be modelled by the paradigmatic Hawk-Dove and minority games. Previous research has highlighted the emergence of fluctuations and limit cycles at the collective level around the mixed equilibrium of the underlying game due to the effect of memory.

Here we zoom in on our analysis and study the properties of the individual’s memory that trigger collective transitions. In particular, we develop a two-faceted description of memory, which includes length and granularity. By analytical and computational means, we show that the precision of the individual’s perception of the outside social environment is an important element determining the transition between synchronous and asynchronous collective states, and between stable trajectories, periodic oscillations and random fluctuations of the group behaviour. Our results confirm that finely grained memories do not necessarily yield evolutionary advantages. We point out why we may expect oscillations to affect real systems, and how individuals may act differently, not because they follow different strategies but due to their own model of the world.
4:00pm - 4:20pm  
**Instability of Homogenous States in the Gray--Scott Model**  
**Joseph Andrew Elmes, Cédric Beaume**  
University of Leeds, United Kingdom  
In this talk, we investigate the instability of spatially homogeneous states in a typical chemical system modelling the reaction and diffusion of two chemical species, U and V. Our study focuses on the Gray--Scott model, a coupled system of PDEs describing the dynamics of chemical concentrations in space and time. The study involves a linear stability analysis of homogeneous states. Changes of stability are identified as functions of key parameters, F and k, where the former is the in-flow rate of U and F-k is the out-flow rate of V. Previous studies have argued that long-wave instabilities of non-trivial homogeneous states in the model are useful when distinguishing between different dynamics attributed to spatio-temporal chaos. Our study contributes to an improved understanding of the linear instabilities that underpin transition to chaos.

4:20pm - 4:40pm  
**Finding NHIM: Identifying High Dimensional Phase Space Structures in Reaction Dynamics using Lagrangian Descriptors**  
**Shibabrat Naik, Stephen Wiggins**  
University of Bristol, United Kingdom  
Computing codimension-1 separatrices and their anchor, normally hyperbolic invariant manifold (NHIM), is the stepping stone in applying phase space transport methods to dynamical systems. Many of these problems give rise to phase space of 4 or more dimensions, and hence geometric approaches become expensive (in time) since a large number of sample initial conditions are required to discretise a volume in phase space. Thus, a practitioner relies on detection methods that are a low dimensional probe of the high dimensional phase space structures. One such method is the Lagrangian descriptor (LD) which encodes geometric property (such as, arc length) of a trajectory at the initial condition on a two-dimensional slice of an isoenergetic hypersurface.

In this talk, we assess the capability of LD for revealing the high dimensional phase space structures that are relevant in chemical reactions. Recent studies have shown that LD plots are versatile, across different models, in locating invariant manifolds that are pathways for reactive trajectories. This calls for a systematic approach to verify that “specific” features in LD plot identify NHIM and codimension-1 separatrices. We discuss this approach in the settings of two and three degrees of freedom Hamiltonian systems where NHIM is known exactly. Then, we present applications to models of chemical reaction where analytical results are unknown.

4:40pm - 5:00pm  
**Roaming reaction dynamics: An invariant manifold perspective**  
**Vladimir Krajnak, Stephen Wiggins**  
University of Bristol, United Kingdom  
For a long time chemical theory stated that dissociation of molecules can only happen in two ways - either the molecule looses an individual atom or it falls apart into smaller molecules. Recent experiments have shown that dissociation of formaldehyde does not follow predictions based on this understanding and a similar behaviour was since reported in a number of other molecules. A third way of dissociation called roaming, in which the molecule takes “a detour”, changed the way we think about chemical reactions. On the example of Chesnavich's model for the reaction $\text{CH}_3^+ \rightarrow \text{CH}_2^+ + \text{H}$, I will explain how roaming can be defined and explained using dynamical systems theory and the geometry of invariant manifolds in phase space.

4:00pm - 5:00pm  
**Contributed Talks 31: Transition to turbulence**  
**Session Chair: Andrew Walton**

4:00pm - 4:20pm  
**Self-sustaining dual critical layer states in plane Poiseuille-Couette flow at large Reynolds number**  
**Rishi Kumar, Andrew Walton**  
Imperial College London, United Kingdom  
The nonlinearity of plane Poiseuille–Couette flow subjected to three-dimensional disturbances is studied asymptotically at large Reynolds number $Re$ based on channel half-width and the maximum velocity of the Poiseuille component. By analysing the nature of the instability for increasing disturbance size $\Delta$, the scaling $\Delta \sim O(R^{\gamma-1/3})$ is identified at which a strongly nonlinear neutral wave structure emerges, involving the interaction of two inviscid critical layers. The striking feature of this structure is that the travelling wave disturbances have both streamwise and spanwise wavelengths comparable to the channel width, with an associated phase speed of $O(1)$. An alternative method to the classical balancing of phase shifts is proposed, involving vorticity jumps, that utilizes a global property of the flow field and enables the amplitude-dependence of the neutral modes to be determined in terms of the wavenumbers and the properties of the basic flow. We present numerical computations of the Rayleigh equation which governs the flow outside of the critical layers shows that neutral solutions exist for non-dimensional wall sliding speeds in the range $0 < V < 2$. It transpires that the critical layers merge and the asymptotic structure referred to above breaks down both in the large-amplitude limit and the limit $V \rightarrow 2$ when the maximum of the basic flow becomes located at the upper wall. We will discuss the new asymptotic structures which emerge in these limits. The talk is based on work to appear in the journal Proceedings of the Royal Society A.
Experiments show that pipe flow can be stabilized by a baffle delaying turbulent transition to and higher [1]. Numerical simulations confirm this effect using a simple model of the baffle [2]. Here we explore the complementary interaction optimization problem of designing a baffle to maximize the energy stability threshold for pipe flow. The baffle is assumed three-dimensional and modelled as exerting a linear drag force, where the baffle “amplitude” is held fixed. The ensuing variational problem is reminiscent of but distinct from the “upper bound” problem of finding the maximal friction factor possible in turbulent pipe flow [3]. We showed that the baffle has to be 1-dimensional due to the solvability condition of the energy stability.

Both the constant pressure gradient and constant mass flux cases are both investigated. The baffle stabilizes the flow more efficiently in the constant pressure gradient case. In both cases, the optimal baffle is localized in the core region.

### 4:40pm - 5:00pm

**Optimizing a baffle to stabilize pipe flow**

*Zijing Ding, Rich Kerswell*

University of Cambridge, United Kingdom

Experiments show that pipe flow can be stabilized by a baffle delaying turbulent transition to and higher [1]. Numerical simulations confirm this effect using a simple model of the baffle [2]. Here we explore the complementary interaction optimization problem of designing a baffle to maximize the energy stability threshold for pipe flow. The baffle is assumed three-dimensional and modelled as exerting a linear drag force, where the baffle “amplitude” is held fixed. The ensuing variational problem is reminiscent of but distinct from the “upper bound” problem of finding the maximal friction factor possible in turbulent pipe flow [3]. We showed that the baffle has to be 1-dimensional due to the solvability condition of the energy stability.

Both the constant pressure gradient and constant mass flux cases are both investigated. The baffle stabilizes the flow more efficiently in the constant pressure gradient case. In both cases, the optimal baffle is localized in the core region.

### 4:00pm - 5:00pm

**Contributed Talks 22: Image processing**

**Session Chair: Paul Shepherd**

**4:00pm - 4:20pm**

**Full Waveform Inversion of Ultrasonic Array Data for Elastic Property Tomography**

*Russell Graeme Niven*

University of Strathclyde, United Kingdom

Ultrasonic phased arrays are being increasingly used in a broad range of industries for non-destructive testing of safety critical structures. The existing flaw imaging methods within the ultrasonic non-destructive community assume that the host material is homogeneous leading to reduced flaw detection and characterisation. Knowledge of the spatial variation in the material’s internal elastic properties would allow for variations in the wave speeds to be accounted for and hence improve flaw imaging. The work presented here endeavours to reconstruct spatially varying wave speed maps of heterogeneous media from ultrasonic phased array data. A 1D semi-analytical model provides a full-waveform forward model for the subsequent inverse problem methodology. A Voronoi tessellation is used to parameterise the material’s structure, where each region is assigned a local wave speed. The objective function is based on a modified Pearson distance and the reversible-jump Markov Chain Monte Carlo (rj-MCMC) method is used to sample the posterior distribution of this function. The reconstructed material map is then used in conjunction with a flaw imaging algorithm and empirical results suggest that this produces more reliable reconstruction of defects.

**4:20pm - 4:40pm**

**Linking reaction-diffusion and threshold dynamics on graphs**

*Jeremy Michael Budd, Yves van Gennip*

Delft Institute of Applied Mathematics, TU Delft, Netherlands

A recent technique in image segmentation and semi-supervised learning has been to study the behaviour of discrete diffusion-driven processes defined on a finite graph. In particular, Bertozzi, Flenner, 2012 developed an algorithm based on the Allen–Cahn reaction-diffusion PDE, and Merkurjev, Kostić, Bertozzi, 2013 developed a similar algorithm using the cheaper Merriman–Bence–Osher threshold dynamics. This interchange of MBO for Allen–Cahn was motivated by their similarity in the continuous context. In this talk, we demonstrate this similarity carries over to the discrete context, and showcase a concrete time-discretisation for Allen–Cahn that yields exactly MBO.

**4:40pm - 5:00pm**

**Robust image segmentation with medical applications**

*Liam Burrow, Ke Chen, Francesco Torella*

Monash University, Melbourne, Australia

This work extends previous problems of a similar kind in incompressible flows. We remark on the challenges of extending the theory to hypersonic non-parallel problems.
Image segmentation is the task of partitioning an image into segments in order to classify and identify objects. It is a popular task in image processing with very important applications, particularly in medical images. Selective segmentation is the aim of identifying an object (or objects) of interest and obtaining an accurate contour representing the position of the object. We will discuss a recent convex segmentation model and mainly focus on its applications for practical use on medical images, with a particular focus on stent tracking in abdominal aortic aneurysms.

4:00pm - 5:00pm
Minisymposium 12B: Modern Approaches to Inverse Problems
Session Chair: Matthias J Ehrhardt

4:00pm - 4:30pm
On support localisation, the Fisher metric and optimal sampling in off-the-grid sparse regularisation.
Clarice Poon
University of Bath, United Kingdom

Sparse regularization is a central technique for both machine learning and imaging sciences. Existing performance guarantees assume a separation of the spikes based on an ad-hoc (usually Euclidean) minimum distance condition, which ignore the geometry of the problem. In this talk, we study the BLASSO (i.e. the off-the-grid version of $\ell^1$ LASSO regularization) and show that the Fisher-Rao distance is the natural way to ensure and quantify support recovery. Under a separation imposed by this distance, we will present results showing that stable recovery of a sparse measure can be achieved when the sampling complexity is (up to log factors) linear with sparsity. On deconvolution problems, which are translation invariant, this generalizes to the multi-dimensional setting existing results of the literature. For more complex translation-varying problems, such as Laplace transform inversion, this gives the first geometry-aware guarantees for sparse recovery. This is joint work with Nicolas Keriven and Gabriel Peyrè.

4:30pm - 5:00pm
Uniqueness of non-negative super-resolution
Jared Tanner
University of Oxford, United Kingdom

Super-resolution is a technique by which one seeks to overcome the inherent accuracy of a measurement device by exploiting further information. Applications are very broad, but in particular these methods have been used to great effect in modern microscopy methods and underpin recent Nobel prizes in chemistry. This topic has received a renewed theoretical interest starting in approximately 2013 where notions from compressed sensing were extended to this continuous setting. The simplest model is to consider a one-dimensional discrete measure $\mu = \sum_{j=1}^k \alpha_j \delta_{t_j}$ which models $k$ discrete objects at unknown locations $t_j$ and unknown amplitudes $\alpha_j$ (typically with non-negative amplitudes). The measurement device can be viewed as a blurring operator, where each discrete spike is instead replaced with a function $\Psi(s, t_j)$ such as a Gaussian $\exp(-|s-t_j|^2/\sigma^2)$, in which case one can make measurements of the form $\psi(s) = \Psi(s, t_j) \alpha_j \delta_{t_j}$. Typically, one measures $m > 2k$ discrete values; that is $\psi(s) = \sum_{j=1}^k \alpha_j \Psi(s, t_j)$. The aim is then to recover the $2k$ parameters $\alpha_j$ and $t_j$ from the $m$ samples and knowledge of $\Psi(s, t_j)$. In this talk we extend recent results by Schiebinger, Robava, and Recht to show that the $2k$ parameters are uniquely determined by their $2k+1$ samples, and that any solution consistent with the measurements within $\pm \frac{\sigma}{\sqrt{2}}$ is proportionally consistent with the original measure. This work is joint with Armin Eftekhari, Andrew Thompson, Bogdan Toader and Hernan Tyagi.

4:00pm - 5:00pm
Contributed Talks 25: Soft matter 2
Session Chair: Christopher Prior

4:00pm - 4:20pm
Writhing of complex entangled tubular bundles
Christopher Prior, Anthony Yeates
Durham University, United Kingdom

Many physical models concern distorted, knotted or entangled tubes. Thin elastic tubes/rods are an example model used in soft matter theory which has been applied to biopolymers, helically coiling plants, ropes, and sea shell growth amongst others. A critical factor in such models is the interplay between internal distortion due the material being twisted and the tube’s global geometry. The Calugareanu theorem links these two through a quantity called the write a measure of the global geometry of the tube’s axis. The sum of write and twist is typically conserved constraining the allowed morphology of the tubes. I shall present work showing how this decomposition can be extended to a far wider variety of domain shapes and also internal field (strain) topologies via a notion of the writhing as the minimally distorted strain field on a domain diffeomorphic to a cylinder. This work has been used to assess the changing connectivity of Magnetic fields but is just as applicable in elastic contexts.

4:20pm - 4:40pm
The Well Order Reconstruction Solution for Three-Dimensional Wells
Giacomo Canevari$^1$, Joseph Harris$^2$, Apala Majumdar$^1$, Yiwei Wang$^3$

$^1$University of Bath, United Kingdom; $^2$Basque Center for Applied Mathematics, Spain; $^3$Illinois Institute of Technology, Chicago, USA
We perform a three-dimensional study on liquid crystal texture inside square wells, within the Landau-de Gennes theory for nematic liquid crystals. We analyse and stimulate the Well Order Reconstruction Solution (WORS) in a three-dimensional setting, first reported by Kralj, S. and Majumdar, A. Order reconstruction patterns in nematic liquid crystal wells. Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences, 2014, 470(2169), 1-18 and analysed by Canevari, G., Majumdar, A. and Spicer, A. Order reconstruction for nematics on squares and hexagons: a Landau- de Gennes study. SIAM Journal on Applied Mathematics, 2017, 77(1), 267-293. The WORS is a 2D pattern which is globally stable for nano-scale square domains, with an optical defect line along both square diagonals. We discuss the relevance of the WORS in a 3D context with realistic boundary conditions, including surface anchoring energies. We prove existence of locally stable critical points with three degrees of freedom and bounds under different temperature regimes in the Landau-de Gennes continuum theory. Using these results, we analyse the stability of a WORS with a constant eigenframe. We then conduct a numerical study of nematic equilibria with finite anchoring on the lateral surfaces of the square well. Numerical studies show that the WORS will no longer exist when the anchoring on the lateral surface is weak enough. We report novel 3D mixed solutions that interpolate between two different 2D solutions across the height of the 3D domain.

4:40pm - 5:00pm

**Indentation tests of two-dimensional materials: separating non-linear material behaviour from experimental error**

**Thomas Graham John Chandler**, Dominic Vella

University of Oxford, United Kingdom

The controlled indentation of thin sheets is an experimental concept used across a range of sciences to extract their material properties. The general idea is that one can extract information on the material properties of the object (e.g. the bending stiffness, Young’s modulus, adhesive force, or pre-tension) from its resistance to being poked. With the recent surge of interest in graphene and other ‘two-dimensional’ materials, this procedure has become especially prevalent but has also led to some controversy: fitted values of graphene’s stretching stiffness vary between 20—700 N/m [more than an order of magnitude difference]. It appears that in some of these measurements, theoretical results have been used inappropriately suggesting that the apparent discrepancy may be, at least in part, due to these errors. Alternatively, this discrepancy may be due to neglected effects such as indenter geometry, non-linear elasticity, sheet bending stiffness and pre-applied stress.

In this presentation, we aim to illuminate and alleviate some of these issues. We will discuss the explicit asymptotic solutions of the force-displacement relation associated with the linear elastic model of typical indentation tests, and determine regions of the parameter space in which they are expected to be valid. We will then consider the effects of material non-linearities, and determine the point at which such effects are expected to become experimentally observable. Finally, we will discuss the consequences of our asymptotic results for the correct implementation of indentation tests in Graphene.

4:00pm - 5:00pm

**Contributed Talks 21: Waves 2**

**Session Chair: Art Gower**

4:00pm - 4:20pm

**Discontinuous Galerkin Method for Viscoelastic Problems with Internal Variables**

**Yongseok Jang**

Brunel University London, United Kingdom

We consider the approximation of wave propagation in viscoelastic media by using spatially Discontinuous Galerkin Finite Element Methods and the Crank Nicolson method in time. A viscoelastic relaxation function is represented by a Volterra integral with a sum of decaying exponential for the kernel. This integro-differential equation is dealt with by introducing two forms of internal variables giving a displacement form and a velocity form, rather than using some technique of quadrature rules. Two fully discrete schemes are defined, which the existence and uniqueness of the solution are shown. In the end, we can prove and observe optimal energy estimates and L2 estimates in space with fixed second order accuracy in time.

4:20pm - 4:40pm

**Waves in Particulate Materials: Beyond Low Frequencies**

**Artur L. Gower**, I. David Abrahams, William J. Parnell

1University of Sheffield; 2University of Cambridge; 3University of Manchester

Particulate materials (powders, composites, emulsions, and gases) are everywhere in nature and industry. Waves, such as sound and light, are ideal to monitor and characterise particulate materials. Yet we still do not fully understand how waves interact with these particles. This is primarily due to multiple scattering and complex interference patterns that appear beyond the low frequency regime. To date, the prevailing method assumes that a wave will perceive the (ensemble averaged) particulate material as a homogeneous medium with one wavespeed and attenuation. However, here I will show that in general, the (ensemble averaged) material has an infinite number of wavespeeds and attenuations all coexisting at the same time. This realisation has answered long standing challenges on modelling wave reflection from particulate materials.

4:40pm - 5:00pm

**P-SV wave scattering from an array of cylinders; tail-end asymptotics for the quasi-periodic Green’s function**

**Georgia Madison Lynott**, I. David Parnell, I. David Abrahams

1University of Manchester, United Kingdom; 2isaac Newton Institute, United Kingdom
We consider the scattering of time-harmonic P- and SV-waves from an infinite periodic array of cylindrical scatterers via the use of boundary element methods and the quasi-periodic Green's function. The slow convergence of the typical quasi-periodic Green's function is well known; we present a novel means of calculation that allows for rapid and accurate approximation of the function. This approach is based on an asymptotic expansion of the summand in the quasi-periodic Green's function in order to derive a tail-end correction term. The tail-end approximation is shown to converge faster than the usual truncation approach, as was recently demonstrated for the acoustic case. This method combined with a boundary element scheme allows us to calculate the transmission and reflection coefficients associated with arrays of cylinders of different cross-sections and varying aspect ratios.

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<td>Mathematics is not border-bound, and this is true in particular for industrial mathematics, as can be seen from the success of the European Consortium for Mathematics in Industry (ECMI). I will briefly sketch the evolution of the so called European Study Group with Industry (ESGI) and a recent collaborative effort: MI-NET, which is funded by the EU Cooperation for Science and Technology (COST). MI-NET has for four years provided a financial support framework to industrial mathematics, supporting ESGIs, STSMs and Industrial Workshops. MI-NET has given a boost to Industrial Maths activities all over Europe, especially in Inclusive Target Countries (ITCs). I will give examples of Industrial Maths problems I have encountered, being a small part of this adventure.</td>
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**Singular Formation in 3D Euler Equations and Related Models**

**Tom Hou**

California Institute of Technology, United States of America

Whether the 3D incompressible Euler equations can develop a finite time singularity from smooth initial data is a long-standing open question in mathematical fluid dynamics.

Recent computations have provided strong numerical evidence that the 3D Euler equations develop a finite time singularity from smooth initial data. I will report some recent progress in providing a rigorous justification of the singularity formation in the 3D Euler equations and related models.

**Nonlinear matrix recovery**

**Florentin Goyens**, **Coralia Cartis**, **Armin Eftekharí**, **Greg Ongie**

1. Oxford, United Kingdom; 2. EPFL, Lausanne; 3. University of Chicago

The field of manifold learning explores ways to find nonlinear structure in a large cloud of data points. It is a very active field of research, and several methods developed in the last decade have already proved to give good results in appropriate settings. On the other hand, there is now established theory for the low-rank matrix completion problem in which one completes a partially observed matrix under the assumption that it is low rank. For this problem there exists recovery guarantees and efficient algorithms. Under sufficient random sampling of the entries, the problem reduces to solving a convex optimization program.

The goal of our project is to complete a partially observed matrix whose columns obey a nonlinear structure. Such matrices are in general full rank, but it is often possible to exhibit a low rank structure when the data is lifted to a higher dimensional space of features. This lifting procedure is performed using a kernel operator. The presence of a nonlinear kernel makes it impossible to write the problem using common matrix completion formulations.

We try to find the best formulation as a nonconvex optimisation problem and see how certain situations allow to leverage existing results from matrix completion theory. Op- timization methods on manifolds and alternative minimization algorithms are explored. We give convergence guarantees and provide numerical results for several test cases.

**Task-adapted reconstruction from tomographic data**

**Carola-Bibiane Schönlieb**

University of Cambridge, United Kingdom

Image reconstruction from indirect measurements, such as they appear in computed tomography (CT) or magnetic resonance imaging (MRI), is often complicated by incomplete and noisy measurements. Lots of work in the mathematical imaging community in the last thirty years or so has gone into the development, analysis and numerical realisation of image reconstruction methods from such data.

While those are classically optimised for some measure of image quality, another strategy is to optimise the image reconstruction for a particular end-task at hand. Such a task-adapted reconstruction strategy is particularly appropriate in most biomedical applications where an image is not reconstructed to look ‘pretty’ but to be used for a subsequent quantification task, e.g. segmentation, classification, motion estimation etc.

In this talk we will discuss several instances of task-adapted reconstruction using variational models as well as recently introduced deeply learned iterative reconstruction approaches. While a variational approach for task-adapted reconstruction gives the advantage of a strong theoretical foundation, its numerical solution and practical application are challenging due to its non convexity and non-smoothness, and dependence on several free parameters. Task-adapted reconstruction with deep learning on the other hand, currently stands on shaky theoretical foundations, however, once trained, renders task adapted reconstruction feasible also for very large-scale inverse problems.

**Bregman algorithms for non-convex optimisation problems with applications in magnetic resonance imaging**


1. Queen Mary University of London, United Kingdom; 2. University College London, United Kingdom; 3. University of Cambridge, United Kingdom; 4. University of Bath, United Kingdom

We propose a unified optimisation framework based on generalised Bregman distances. We discuss theoretical properties of the framework and give convergence guarantees for both convex and nonconvex optimisation problems. We conclude with numerical results for industrial and medical applications in magnetic resonance imaging.
Empirical networks. We find that tuning the properties of the examined users to be examined. For instance, there is in node dynamics, network structure, and sentiment? To this end, we examine the relationship between social structure and sentiment through the analysis of a large collection of tweets about the Irish Marriage Referendum of 2015. Using the sentiment of these tweets, we construct networks to aggregate sentiment and use it to study the interactions among users. Our results show that the sentiment of mention tweets is correlated between users, and there are significantly more connections between users with similar sentiment scores than among users with opposite scores. Using this sentiment based homophily, we were able to classify users as either yes or no aligned supporters with high accuracy between users with similar sentiment scores than among users with opposite scores. Using this sentiment based homophily, we were able to classify users as either yes or no aligned supporters with high accuracy.

Chimera states are characterised by the symmetry breaking on homogeneous systems of identical dynamical units, under very special conditions. While the phenomenon has been largely investigated in the recent years, the identification of chimera in real system has been more intricate. Indeed, the very constrained conditions required for chimera states to emerge are rather unexpected in real systems, which tend to be noisy and made of non-identical units. Here, we study the collective dynamics of modular networks with heterogeneous properties, resembling the diversity found in empirical networks. We find that tuning the properties of the underlying modular structure leads to a variety of dynamical behaviours, including a different mechanism for the emergence of chimera-like states at a phenomenological level.

Efflux pumps are an essential mechanism for bacteria that can account for antibiotic resistance. If an efflux pump can expel an antibiotic so that its concentration within the cell is below a killing threshold the bacteria can become resistant to the antibiotic. Efflux pumps may be specific or they may pump various different substances and compounds. The latter is one main reason that many efflux pumps are linked with multi drug resistance (MDR). In particular over expression of the AcrAB−TolC efflux pump system is commonly linked with MDR in both E. coli and Salmonella. We look at the complex gene regulation network that controls

1. Center for Brain Cognition, Pompeu Fabra University, Spain; 2. Namur Institute for Complex Systems (naxys), Department of Mathematics, University of Namur, Belgium; 3. Institute of mathematical sciences and computation, University of Sao Paulo, Brazil.

1. University of Oxford; 2. Sinnia, Mexico City; 3. MACSI, Department of Mathematics and Statistics, University of Limerick.

Twitter has been studied as an open and popular venue for the spreading of information and facilitation of debate. The accurate identification of the sides of a debate is fundamental to this. In this talk, we will aim to answer the question: Is it possible to identify mutually positive and antagonistic relationships between groups, and understand how they interact with each other using network structure and sentiment? To this end, we examine the relationship between social structure and sentiment through the analysis of a large collection of tweets about the Irish Marriage Referendum of 2015. Using the sentiment of these tweets, we construct networks to aggregate sentiment and use it to study the interactions among users. Our results show that the sentiment of mention tweets is correlated between users, and there are significantly more connections between users with similar sentiment scores than among users with opposite scores. Using this sentiment based homophily, we were able to classify users as either yes or no aligned supporters with high accuracy (89%). This allowed for the interactions of ideologically opposed users to be examined. For instance, there were numerous conversations between users on opposing sides of the debate in the absence of follower connections, which suggests that there were efforts by some users to establish dialogue and debate across ideological divisions. These results have potential applications in the integration of data and meta-data to study opinion dynamics, public opinion modelling, and polling.

Efflux pumps are an essential mechanism for bacteria that can account for antibiotic resistance. If an efflux pump can expel an antibiotic so that its concentration within the cell is below a killing threshold the bacteria can become resistant to the antibiotic. Efflux pumps may be specific or they may pump various different substances and compounds. The latter is one main reason that many efflux pumps are linked with multi drug resistance (MDR). In particular over expression of the AcrAB−TolC efflux pump system is commonly linked with MDR in both E. coli and Salmonella. We look at the complex gene regulation network that controls

1. University Of Birmingham, United Kingdom; 2. University Of Nottingham, United Kingdom

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expression of genes central to controlling the efflux pump genes acrAB and acrEF in Salmonella. By using mathematical modelling, we represent this gene regulatory network as a model in the form of a system of ordinary differential equations (ODEs). Using time dependent asymptotic analysis, we can examine in detail the behaviour of the efflux system on various different timescales. By obtaining asymptotically approximated steady states, we are then able to look into various different methods to inhibit efflux pumps to counter MDR.

11:20am - 11:40am
Equilibria and oscillations of a regulated two--gene model
Gabor Kiss
Queen's University Belfast, United Kingdom

We investigate the number of equilibria and the dynamics of a two--gene system with an autoregulatory feedback loop. We show that the number of equilibria of the studied planar system of non--linear ordinary differential equations depends on the system parameters. We also provide numerical evidence for bistability, the existence unstable periodic orbits and indicators of existence of orbits homoclinic to an equilibrium. Finally, we partially describe the effects of time delay on the dynamics.

11:40am - 12:00pm
Modelling human embryonic stem cell colonies to optimise clonality
Laura Wadkin¹, Sirio Orozco-Fuentes¹, Irina Neganova², Sanja Bojic¹, Nick Parker¹, Anvar Shukurov¹, Majlinda Lako¹
¹Newcastle University, United Kingdom; ²Institute of Cytology, RAS, Russia

Human embryonic stem cells, hESCs, hold great promise for developments in regenerative medicine and are at the forefront of modern biological research due to their ability to differentiate into any type of human adult cell and their potential to self-renew indefinitely through repeated divisions. Clinical applications often rely on homogeneous cell populations originating from a single cell. As part of an interdisciplinary team at Newcastle University, I am working to optimise experiments by modelling the behaviour of hESC colonies using a combination of agent-based and stochastic techniques. Having already extracted parameters of stem cell kinematics, we now focus on colony proliferation and optimising clonality. Using bespoke experiments from our group, we unexpectedly found colony populations to be multimodal, associated with different numbers of founding cells. This can be predicted by considering cell-cell interactions on randomly seeded cells. We have developed a multi-population stochastic exponential model for the proliferation of hESCs which captures our experimental observations and can be used as a predictive tool to achieve the best outcome for homogeneous clonal colony growth from different seeding densities.

12:00pm - 12:20pm
Understanding Shh Aggregation through Mathematical Modelling
Daniel Derrick¹, Kathryn Wolton², Richard Currie², Marcus Tindall¹,3
¹Department of Mathematics and Statistics,The University of Reading, United Kingdom; ²Syngenta, Jealott's Hill International Research Center, Berkshire, United Kingdom; ³Institute of Cardiovascular and Metabolic Research, University of Reading, United Kingdom

Effective regulation of the sonic hedgehog (Ssh) signalling pathway is essential for the development of a wide variety of species. Dysregulation of the pathway is associated with the occurrence of developmental malformations. Shh signalling involves the formation of Shh aggregates on the surface of producing cells which subsequently diffuse towards receiving cells located elsewhere in the developing embryo. Various mechanisms have been postulated regarding how Shh aggregates form and their role in the overall signalling process. In this talk we present a mathematical model, formulated using the theory of nonlinear ordinary differential equations to explore three proposed mechanisms of Shh aggregation: multimerisation and association with heparan sulfate proteoglycan (HSPG) or lipoproteins. Our results demonstrate that the size distribution of Shh aggregates formed resembles the shape of a gamma distribution, a result in agreement with previous experimental data. We find that the gamma distribution shape is robust to parameter changes, and subsequently, also to variations in the processes by which Shh is recruited by HSPGs and lipoproteins. This work demonstrates that the timescale of formation of different sized Shh aggregates is likely to play an important role in Shh diffusion and will be strictly regulated during vital developmental periods.

11:00am - 12:30pm
Minisymposium 19B: Different Viewpoints on Multi-Scale Problems
Session Chair: Hong Duong
Session Chair: Johannes Zimmer

11:00am - 11:30am
Averaging of fast-slow Hamiltonian systems
Matthias Klar, Karsten Matthies, Johannes Zimmer
Bath University, United Kingdom

Fast-slow Hamiltonian systems can be seen as toy models of molecular dynamics, where the two-scale nature models the scale separation leading to thermodynamic behaviour. In this talk I will analyse a fast-slow Hamiltonian system of two oscillating particles. The aim is to understand how the microscopic oscillations translate into thermodynamic expressions in an averaged (effective, macroscopic) model. I will present a two-scale expansion, both through asymptotic expansion and two-scale convergence. A particular focus of the talk will be on how the first and second law of thermodynamics appear on a coarse-grained level.

11:30am - 12:00pm
Front propagation in periodic flows
A classical model for the concentration of spreading reacting chemical is the Fisher--Kolmogorov--Petrovskii-Piskunov-type model. Numerous environmental and engineering applications, from the dynamics of ocean plankton to combustion, motivate its extension to include the effect of an incompressible background periodic fluid flow. In the long-time limit, a steadily propagating pulsating front is established. We will describe how a multi scale theory of large deviations can be used to provide its average speed of propagation for arbitrary molecular diffusivity (Peclet number) and reaction rate (Damkohler number). We will show that its value can be obtained by solving an eigenvalue problem and use asymptotic methods to express it explicitly in various regimes. We will finally contrast the sharp front obtained in the limit of large Peclet and Damkohler numbers against its heuristic approximation by the G equation.

12:00pm - 12:30pm

On using fluctuation dissipation relations for finding macroscopic evolution equations from particle observations

Peter Embacher1, Nicolas Dirr1, Johannes Zimmer2, Celia Reina4, Xiaoguai Li1
1University of Warwick, United Kingdom; 2Cardiff University, United Kingdom; 3University of Bath, United Kingdom; 4University of Pennsylvania, USA

A method is presented to use observations of particle fluctuations to computationally ex-tract the thermodynamic metric in macroscopic evolution equations of gradient flow type along the entropy. For this we consider particle systems in local equilibrium, which exhibit Gaussian fluctuations. Entropy-driven gradient flows have attracted much theoretical attention as alternative ways to represent the dynamics of a variety of dissipative systems. The new approach uses them to characterise the evolution equations of these systems from observation data, thus making this concept more accessible for applications.

11:00am - 12:30pm

Minisymposium 18B: Modelling stochastic biological systems
Session Chair: Cameron Andrew Smith
Session Chair: Kit Yates

11:00am - 11:30am

Homogenization approximations for advection-dominated solute transport in a spatially disordered domain

George Price, Oliver Jensen
The University of Manchester, United Kingdom

Solute transport in nature often takes place in spatially complex domains with inherently random structures. To evaluate the effects of stochastic variability, we study a simple model involving unidirectional flow past a one-dimensional array of randomly located point sinks, which remove solute via first order kinetics. We focus on the case where advection dominates diffusion, which causes concentration fields to become non-smooth, with boundary layers forming upstream of each sink. We extend a homogenization approximation (Russell & Jensen,IMA J. Appl. Math. 2019, hzx004) using a Green's function method to evaluate corrections arising due to discrete and disordered sink locations, which is tested against Monte Carlo simulation. The solute field develops a staircase structure, with (co)variances that are either smooth or exhibit spikes, depending on the degree of disorder in sink locations. This approach allows us to characterise uncertainty in net solute transfer in models of physiological transport.

11:30am - 12:00pm

Modeling molecular diffusion in the intracellular environment

Remus Stana
University of Leeds, United Kingdom

Many cells of the immune system have receptors which are produced in the nucleus and these move under the influence of diffusion until they reach the outer membrane of the cell. Depending on the type of receptor, they might also diffuse on the surface of the cell until either a certain period of time has passed or the receptor encounters a peptide. After either of these events the receptors re-enter the cytoplasm and diffuse until they are absorbed by the nucleus. We are interested in the first passage properties of the receptors. Particularly, two quantities of great importance are the mean time T from creation of a receptor to its absorption back into the nucleus and the distribution of eventual hitting points on both the nucleus and the cytoplasm. We show how these quantities can be determined explicitly for two types of geometry, namely when the nucleus and membrane are concentric and eccentric, both in 2D and 3D. For this purpose, we derive an analytic expression for the Green's function of the Laplace equation for a domain bounded by non-concentric surfaces in two dimensions and three dimensions subject to absorbing outer surface and reflecting inner surface and vice versa. Utilizing the Green's function we derive an expression for T and compare with previous results in the literature. Furthermore, using the Green's function we calculate exact formula for the distribution of eventual hitting points and compare it with numerical results.

12:00pm - 12:30pm

Stochastic dynamics and regulation of Filopodia-like structures

Ulrich Dobramysl1,2, Iris Jarsch1,2, Hanae Shimo1,2, Yoshiko Inoue1,2, Benjamin Richier1,2, Jonathan Gadby1, Julia Mason1, Astrid Walrant1, Richard Butler1, Edouard Hannezo1, Benjamin Simons1,2, Jennifer Gallop1,2
1Wellcome Trust / CRUK Gurdon Institute, University of Cambridge, UK; 2Department of Biochemistry, University of Cambridge, UK; 3Institute of Science and Technology Austria, Austria; 4Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK
Filopodia are finger-like cell protrusions that are rich in the cytoskeletal filament-forming protein actin. To understand how the diverse set of proteins involved in the regulation of actin (de-)polymerization gives rise to the observable dynamics of filopodia, we employed a cell-free assay that generates filopodia-like structures (FLS). By tracking the localisation of regulatory proteins and the morphology of FLS over time using confocal fluorescence microscopy, we find that FLS growth is a stochastic process and that the growth velocity approximately follows a Laplace distribution. Using the algebra of random variables, we were able to show that such a Laplace-like distribution can be constructed from the sums of products of normally distributed numbers. This allowed us to link the fluctuations in the abundance of regulatory proteins to the growth dynamics of FLS via stochastic modelling and match the observed length and growth persistence time distributions. Our results explain how heterogeneous sets of regulatory proteins can interact to produce universal growth behaviour.

**Minisymposium 20B: Understanding the dynamics of particle and droplet impacts**

Session Chair: Ryan Palmer  
Session Chair: Frank Thomas Smith

**11:00am - 11:30am**

**Three-dimensional gas-cushioned droplet impacts with finite-depth liquid layers**

**Peter Daniel Hicks**  
University of Aberdeen, United Kingdom

The influence of gas-cushioning in three-dimensional droplet impacts with liquid layers will be investigated in a coupled viscous gas and inviscid liquid regime. Green’s identity will be used to derive a boundary integral equation relating the vertical acceleration of the liquid free-surface to the pressure at the liquid interface. This will be coupled to a viscous squeeze film equation governing the gas behaviour, and the resulting coupled system of integro-differential equations will be solved numerically. It will be shown that the impermeable base of the liquid layer influences gas cushioning when the depth of the liquid layer is comparable to the horizontal extent of the gas cushion. Limits corresponding to deep and shallow water will be explored. The boundary integral equation will be expressed in terms of two-dimensional Fourier convolutions and the use of Hankel and Fourier transforms to calculate efficiently the free-surface evolution in axisymmetric and three-dimensional droplet impacts will be discussed. The effect of different surface tension coefficients on the droplet and liquid layer free-surfaces will be described.

**11:30am - 12:00pm**

**Fluid-body interactions and impacts at high flow rates**

**Frank Thomas Smith**  
UCL, United Kingdom

This presentation discusses recent work on dynamic fluid-body interactions and related features of impacts in boundary layers, channels and films. The research is based on analysis and corresponding reduced computational investigations for high flow rates. The work includes relatively small bodies, inside or close to a viscous-inviscid wall layer or an inviscid wall layer typically in a two-dimensional configuration, as well as considering larger bodies. The typical body motion and fluid motion in these settings are taken to affect each other comparably, in a two-way coupling, for general application. Of special interest are the properties for thin bodies representing ice shards of various shapes and sizes and their impacts on solid surfaces or on water films.

**12:00pm - 12:30pm**

**Towards High-speed Impacts on Engineered Surfaces**

**Manish K Tiwari**  
Nanoengineered Systems Laboratory, University College London, United Kingdom

Impact of liquid and solid objects has widespread relevance in nature and man made applications. In this current talk, I will focus on design of nanoengineered surfaces with impact resistance as the key guiding criteria. In particular, I will discuss features of liquid impact, impalement resistance of micro/nanoengineered surfaces, and how these features can be coupled rationally with acoustic features to improve performance. High-speed imaging of droplets and jets impacting on various superhydrophobic and impact resistant surfaces will be presented and discussed. Outstanding challenges, both from theoretical and experimental perspective, will be touched upon through out the presentation to provide a personal perspective on the way forward in this field.

**11:00am - 11:20am**

**Primary blast lung injury simulator: a mathematical/computational modell based on Human Data**

**Mainul Haque**, **Timothy Scott**

1University of Portsmouth, UK.; 2The Royal Stoke Hospital UK.

Mathematical modeling and computational simulation are important tools in medicine where in vivo studies are expensive, difficult or impractical. Primary blast lung injury (PBLI) is the most important component of a multisystem syndrome of injury that results from exposure to an explosive shockwave. The majority of such casualties require ventilation in an intensive care unit Due to the complexities of representing the parameters of PBLI, modeling the clinical outcomes is challenging. However, computational modeling may provide considerable insight into improving the understanding and treatment of PBLI. The aim of this paper is to provide a brief outline of a PBLI simulator developed by our group, its initial validation using Human/animal data.
data. The simulator described in this paper can accurately model primary blast lung injury as well as the potential effect of a range of medical interventions. We describe the use of a novel primary blast lung injury simulator to evaluate the potential efficacy of continuous positive airway pressure in 6 in-silico casualties over 24 hours after injury. Our results suggest that primary blast lung injury is a form of acute lung injury that can be effectively managed with continuous positive airway pressure. In austere environments or in circumstances where medical resources are overwhelmed, continuous positive airway pressure using ambient air may be of benefit. This study provides a detailed message to the clinicians which guide the clinicians to decide optional ventilation strategies for the patients with PBLI.

11:20am - 11:40am

New information from old signals: A novel approach to the analysis of ECG waveforms

Jane V Lyle1, Philip J Aston1, Manasi Nandi2
1Department of Mathematics, University of Surrey, United Kingdom; 2Faculty of Life Sciences and Medicine, King's College London, United Kingdom

Proactive ECG monitoring is increasingly common, but generates large quantities of data with the need to derive diagnostic and predictive information. Heart rate variability (HRV) and the identification of particular points on the ECG wave remain the mainstay of analysis. However, both techniques exclude the wealth of information in the waveform profile, and any subsequent categorisation of nonlinear features does not provide specific morphological detail.

We describe a new approach for extracting information from any approximately periodic waveform, and how this can be applied to the challenge of analysing ECG signals which are irregular, non-stationary and often noisy. From a single lead ECG measurement, we use Takens' method of delay coordinates to reconstruct an attractor in three dimensional phase space. Projecting the attractor on to a plane allows us to reduce baseline wander in the signal, whilst retaining all of the information in the shape of the underlying waveform.

We then apply machine learning to features extracted from the attractor to show the potential biological relevance of our technique. We illustrate this by distinguishing the presence or absence of a mutant gene using mouse ECG signals and demonstrating significant gender differences in the human ECG that have not previously been so clearly discriminated.

This novel analysis of ECG signals uses the attractor properties to derive useful clinical information from biological big data, providing a basis for supporting a personalised approach to early detection, diagnosis and treatment of a range of diseases.

11:40am - 12:00pm

Revealing hidden mutations in intestinal tissue

Doran Khamis, Ed Morrissey
University of Oxford, United Kingdom

The transition to malignancy in intestinal tissue is caused by the build-up of genetic mutations in the stem cells of intestinal crypts. Certain mutations cause abnormal cell dynamics, increasing turnover rate and driving effects that cascade upwards in scale and lead to the spatial expansion of the mutant through the process of crypt fission. Large patches of mutant tissue can thus form, and patches containing particularly pernicious mutations act as staging areas for the transition to colorectal cancers. We investigate the patchy spatial structure of intestinal tissue and predict, through a combination of Bayesian modelling and deep neural networks, the location of "hidden" mutant patches.

12:00pm - 12:20pm

Modelling induced drug resistance to enzalutamide in the TRAMP model of prostate cancer.

Marianna Cerasuolo1, Alessia Ligresti2, Roberto Ronca2
1University of Portsmouth, United Kingdom; 2University of Brescia, Italy; 3National Research Council of Italy, Italy

Androgen deprivation therapy ability to reduce tumour growth represents a milestone in prostate cancer treatment, nonetheless most patients eventually become refractory and develop castration-resistance prostate cancer (CRPC). Enzalutamide is a second-generation drug recently approved for the treatment of CRPC. However, cases of tumour resistance to enzalutamide have now been reported. In this study the multistage model of TRAMP mice and TRAMP-derived cells have been used to extensively characterise in vitro and in vivo response and resistance to second-generation androgen receptor antagonist enzalutamide.

Within the study a multiscale mathematical model has been developed. The set of six stochastic differential equations describes the interaction between heterogeneous cancer cell populations, the pharmacokinetics of the administered drug and the dynamics of the tumour microenvironment. The integration of experimental data with a mathematical framework of tumour growth allowed to gain insights into the dynamics of intratumoral evolution. The response of prostate cancer to different therapy strategies was explored with in silico experiments. The model clearly shows that the use of enzalutamide does always cause the onset of resistance and that no strategy allows to successfully control the disease, suggesting the need of drug combination therapies.
In this talk we present a framework for estimating parameters in macroscopic models for crowd dynamics using data from individual trajectories. We consider a model for the unidirectional flow of pedestrians in a corridor which consists of a coupling between a density dependent stochastic differential equation and a nonlinear partial differential equation for the density. In the stochastic differential equation for the trajectories, the velocity of a pedestrian decreases with the density according to the fundamental diagram. Although there is a general agreement on the basic shape of this dependence, its parametrization depends strongly on the measurement and averaging techniques used as well as the experimental setup considered. We will discuss identifiability of the parameters appearing in the fundamental diagram, introduce optimisation and Bayesian methods to perform the identification, and analyse the performance of the proposed methodology in various realistic situations. Finally, we discuss possible generalisations, including the effect of the form of the fundamental diagram and the use of experimental data.

11:30am - 12:00pm
Learning a Sampling Pattern for MRI

Ferdia Sherry¹, Matthias J. Ehrhardt², Carola-Bibiane Schönlieb³

¹University of Cambridge; ²University of Bath

The discovery of the theory of compressed sensing brought the realisation that many inverse problems can be solved satisfactorily even when measurements are incomplete. This is particularly interesting in an imaging modality such as magnetic resonance imaging (MRI), where long acquisition times are problematic. The measurements taken in MRI are often modelled as samples of the Fourier transform of the signal to be recovered. In this work, we consider the problem of learning a sparse sampling pattern that can be used to obtain high quality reconstructions for images that are similar to the images used in training, while only having to sample along the learned sampling pattern. The approach that is taken is that of bilevel learning: a minimisation problem is solved, which has constraints that are formulated as the solution to variational regularisation problems (the problems that are solved to reconstruct a signal from measurements). The framework that we set up for learning a sampling pattern allows a sampling pattern of scattered points or of cartesian lines in k-space to be learned and can easily be extended to other parametrisations of the sampling pattern.

12:00pm - 12:30pm
Learned image reconstruction for high-resolution tomographic imaging

Andreas Hauptmann

University of Oulu, Finland

Recent advances in deep learning for tomographic reconstructions have shown great potential to create accurate and high quality images with a considerable speed-up of reconstruction time. In this talk I will discuss two common approaches to combine deep learning methods, in particular convolutional neural networks (CNN), with model-based reconstruction techniques. These approaches are illustrated with two conceptually different imaging modalities:

- For accelerated dynamic cardiovascular magnetic resonance we can train a CNN to remove noise and aliasing artefacts from an initial reconstruction to obtain clinically useful information. For the more challenging problem of limited-view photoacoustic tomography, we rather need to train a network that performs an iterative reconstruction which feeds back the model information into the reconstruction algorithm to successively negate limited-view artefacts.

11:00am - 12:30pm
Minisymposium 16B: Toy mathematical models in the physical sciences

Session Chair: Philippe Trinh

11:00am - 11:30am
A toy model for bacterial nutrient uptake

Mohit Dalwadi¹,², Yanming Wang², John King²,³, Nigel Minton²

¹Mathematical Institute, University of Oxford; ²Synthetic Biology Research Centre, University of Nottingham; ³School of Mathematical Sciences, University of Nottingham

In mathematical models that include nutrient delivery to bacteria, it is prohibitively expensive to include many small bacterial regions acting as volumetric nutrient sinks. To combat this problem, such models often impose an effective uptake instead. However, it is not immediately clear how to relate properties on the bacterial scale with this effective result. For example, one may intuitively expect the effective uptake to scale with bacterial volume for weak uptake, and with bacterial surface area for strong uptake.

I will present a general model for bacterial nutrient uptake, and upscale the system using homogenization theory to determine how the effective uptake depends on the microscale bacterial properties. This will show us when the intuitive volume and surface area scalings are each valid, as well as the correct form of the effective uptake when neither of these scalings is appropriate.

11:30am - 12:00pm
A toy model for the manufacture of liquid crystal devices

Joseph R. L. Cousins, Stephen K. Wilson, Nigel J. Motttram

Department of Mathematics and Statistics, University of Strathclyde, United Kingdom

Liquid crystal devices (LCDs) are ubiquitous in modern day life, and faster and more accurate manufacture of these devices is required to meet increasing global demand. The optimisation of the manufacturing process generally involves attempting to reduce manufacturing time by increasing flow velocities and filling speeds.
However, implementing such changes runs the risk of causing deformation to the director structure which is crucial to the display.

A common process of filling the liquid crystal layer in LCDs used by display manufacturers is the One-Drop-Filling (ODF) process. In the first stage of the ODF process, a bottom substrate is coated with an alignment layer in order to correctly orient the liquid crystal layer within the cell. Droplets of liquid crystal are then dispensed onto the bottom substrate and are allowed to equilibrate. In vacuum, a top substrate is then lowered at a constant speed onto the droplets, squeezing them, causing them to coalesce, and eventually creating a continuous thin film of liquid crystal within the cell. Finally, the cell is cured and sealed to make it ready for use in LCDs. Although this method is an efficient way to fill liquid crystal cells used in LCDs, it is known that it can cause deformation to the director structure within the liquid crystal cells known as “ODF mura” which, in turn, can affect the optical performance of the final display.

We propose a toy model for the coalescence of droplets during the squeezing stage of the ODF process to provide insight into the formation of this ODF mura. This toy model assumes that the timescale for changes in the shape of droplets due to surface tension is much longer than that of squeezing, and so the effects of surface tension can be neglected. This assumption allows the calculation of the spreading behaviour of multiple squeezed droplets to be determined by geometrical methods using conservation of volume.

We obtain implicit expressions for the droplet boundary speed of multiple coalescing droplets which allow us to make direct comparisons with experimental photographs of the ODF mura. Specifically, the deformation to the director structure at any point is assumed to be proportional to the droplet boundary speed as it passes over that point. The deformation to the director structure calculated shows a remarkable similarity to experimental photographs of the ODF mura. Motivated by the success of this toy model we further investigate the flow and director within a single droplet during squeezing using Ericksen-Leslie continuum theory.

12:00pm - 12:30pm
A toy model for surge in turbochargers
Kate Powers
University of Bath, United Kingdom

Turbochargers increase the power output of engines, meaning that smaller (and hence greener) engines can be used in vehicles. Surge is an instability that arises when there is not enough air passing through the turbocharger compressor. Operation in surge results in pressure and mass flow oscillations that are often damaging to the compressor and its installation. Therefore, predicitng the location of surge onset is important for turbocharger manufacturers and engine designers.

In this talk, I will describe a new 1D modelling approach for surge that was developed using compressible, rotating, Navier-Stokes equations. I will discuss the motivation behind developing a new approach, and provide some validation of the model through comparison to experimental data.

11:00am - 12:30pm
Contributed Talks 8: Fluids 4
Session Chair: Guanglian Li

11:00am - 11:20am
Spatio-temporal symmetry-breaking of the flow past an oscillating cylinder
Puneet Matharu, Andrew Hazel, Matthias Heil
University of Manchester, United Kingdom

At a sufficiently large Reynolds number the flow around a stationary cylinder results in the formation of the famous von Kármán vortex street – a time-periodic flow in which vortices are shed, alternately on either side of the cylinder. When the cylinder performs forced oscillations transverse to the flow direction, the vortex shedding pattern becomes significantly more complex, leading to the formation of so-called "exotic wakes" whose character is controlled by the Reynolds number as well as the frequency and the amplitude of the cylinder’s motion (Williamson & Roshko 1988). The question we wish to address is this: do these different patterns arise via (i) a continuous change in vorticity pattern (with quantifiable discrete changes to its topology) in a "complicated" flow or; (ii) via bifurcations of the underlying solutions of the Navier-Stokes equations?

We compute the time-periodic flow past an oscillating cylinder and show that the transition from the so-called 2S (associated with the shedding of two single regions of vorticity per cylinder oscillation) to the P+S wake mode (associated with the shedding of a pair of vortices and single region of vorticity per cylinder oscillation), which occurs at $A^* = A_{wr}$, arises through a spatio-temporal symmetry-breaking supercritical pitchfork bifurcation of the time-periodic solution (i.e. scenario (ii)). This implies that for values of $A^* > A_{wr}$ the 2S solution still exists but is unstable.

11:20am - 11:40am
Talk cancelled

11:40am - 12:00pm
Generation of first Mack modes in supersonic boundary layers by slow acoustic waves interacting with streamwise isolated wall roughness
Yinhui Liu1, Ming Dong1, Xuesong Wu2
1The centre for High-speed Aerodynamics Research, Tianjin University, Tianjin 300072, China; 2Imperial College London, 180 Queen’s Gate, London SW7 2AZ, UK
This paper investigates the receptivity of a supersonic boundary layer to slow acoustic waves whose characteristic frequency and wavelength are on the triple-deck scales, and hence the phase speed is asymptotically small. Acoustic waves on these scales are of special importance as they have the interesting property that an O(1) perturbation in the free stream generates much larger, O(R1/8), velocity fluctuations inside the boundary layer. Their interaction with a streamwise localised roughness element leading to stronger receptivity is studied using triple-deck theory and direct numerical simulations (DNS) in supersonic boundary layer. The receptivity coefficient, defined as the ratio of the streamwise-velocity amplitude of the excited instability wave to that of the free stream incident acoustic wave, serves to characterize receptivity efficiency. Its dependence on the width of the roughness, Reynolds number, incident angle and frequency of acoustic wave is investigated. The results show that the theoretical predictions are in reasonable agreement with the DNS results when the roughness element is located near the lower branch of the instability. A roughness element with a fixed height produces the strongest impact when its width is comparable with the instability wavelength. The behaviour of the theoretical solutions obtained for R → ∞ holds at finite Reynolds numbers. The receptivity is sensitive to the incident angle or the phase speed of the acoustic wave. The receptivity coefficient is proportional to the peak amplitude of the u-component of the acoustic wave inside boundary layer.

12:00pm - 12:20pm
The periodic multiply-connected Schwarz-Christoffel mapping
Peter Jonathan Baddoo¹, Darren G Crowdy²
¹University of Cambridge, United Kingdom; ²Imperial College London, United Kingdom

Schwarz-Christoffel (S-C) formulae provide conformal mappings from circular domains to polygonal domains. Consequently, they are important tools for applied mathematicians seeking to solve problems involving complicated geometries. We present a major extension to previous S-C mappings by permitting the target domain to consist of a periodic array of polygons. Moreover, by employing the transcendental Schottky-Klein prime function, the new S-C formula is valid for any number of polygons in each period window. We demonstrate several examples of the new mapping for a range of connectivities and show that, when coupled with the “new calculus of two-dimensional vortex dynamics”, the new S-C mapping is a powerful tool for the study of fluid flows in periodic domains. Finally, we formulate the accessory parameter problem of determining the pre-vertices and conformal geometry in the canonical domain in order to achieve the desired target domain.

11:00am - 12:30pm
Contributed Talks 11: Droplets 3
Session Chair: Alexander Wray

11:00am - 11:20am
Competitive evaporation of multiple sessile droplets
Stephen K. Wilson, Alexander W. Wray, Brian R. Duffy
University of Strathclyde, United Kingdom

An asymptotic model is derived for the competitive diffusion-limited evaporation of multiple thin sessile droplets under the assumption that the droplets are well separated. Comparisons are made with numerical solutions of the full governing equations in order to verify the accuracy of the model; in particular, the model is found to perform well even outside its anticipated range of applicability, up to and including the limit of touching droplets. The “shielding” effect of other droplets is demonstrated, and the model is used to investigate the effect of this shielding on droplet evolutions and lifetimes, as well as on the coffee-ring effect.

11:20am - 11:40am
Bifurcation analysis of evaporating droplets on smooth surfaces
Michael Ewetola, Marc Pradas
The Open University, United Kingdom

Droplet evaporation is important in many processes including ink-jet printing, micro-patterning, coating, and cooling. In this study, the behaviour of a two-dimensional droplet that is slowly evaporating on a solid surface due to mass diffusion is investigated. We consider surfaces that have smooth periodic variations and make use of bifurcation theory to analyse the stability properties of the system as the volume of the droplet is changing in time. We observe that a hierarchy of bifurcations is triggered by the underlying properties of the surface, including pitchfork and saddle-node bifurcations. The bifurcation points, which can be predicted theoretically, correspond to critical volumes at which the droplet may change location by shifting laterally. A predictable direction for the droplet movement is also determined when the chemical variation is asymmetric, which could be significant for designing, e.g., self-cleaning surfaces. In addition, we make use of a diffuse interface formulation to study the dynamics of the droplet as it evaporates, observing a sequence of events in which the droplet base radius, contact angle, and mid-point rapidly change, in agreement with the theoretically predicted bifurcation points.

11:40am - 12:00pm
A 2D model for the evaporation of a pair of liquid ridges
Feargus Schofield¹, Stephen Wilson¹, David Pritchard¹, Alexander Wray¹, Khellil Sefiane²
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Understanding the dynamics of sessile liquid droplet evaporation on solid substrates is critical for many industrial processes, such as ink-jet printing, coating, and spray cooling, as well as for drug delivery systems and chemical spill containment. Consequently, in recent years there has been a rapid growth of scientific interest in all aspects of droplet evaporation, including determining the lifetimes of evaporating droplets. Much of the previous theoretical work has focused on the evaporation of a single droplet. However, there is very
little research which captures the physics of the neighbouring evaporating droplets which are present in almost all industrial processes. In the present work to provide insight into the 3D problem for a pair of neighbouring droplets we investigate the equivalent 2D problem for a pair of neighbouring liquid ridges. We use conformal mapping techniques to investigate the 2D problem of an evaporating ridge of liquid. We then extend the single ridge model to include an identical neighbouring ridge of liquid and obtain analytical expressions for the evaporative flux from the ridges. From this analysis we observe the so-called “shielding effect”, in which the atmosphere between the ridges becomes more concentrated with vapour thus dampening the evaporative flux into this region. From the evaporative flux of the ridges we obtain analytical expressions for the evaporation rates, and hence the lifetimes, of the ridges in various modes of evaporation. In particular, we show that decreasing the distance between the neighbouring ridges will increase the magnitude of the shielding effect thus leading to longer lifetimes.

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12:00pm - 12:20pm

**Evaporation of a sessile droplet in a shallow well**


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The evaporation of sessile droplets occurs in a wide variety of physical contexts, with numerous applications in nature, industry and biology. Examples of real life applications include blood splatter in forensic science, DNA mapping and gene analysis in the medical industry, the spreading of pesticides on leaves, and coating technologies. In particular, the evaporation of droplets plays a key role in inkjet printing used in the manufacture of OLED displays. In this talk I will formulate and analyse a mathematical model for the evolution of a thin droplet undergoing diffusion-limited evaporation on a non-uniform substrate, specifically in an axisymmetric well of the kind often encountered in OLED manufacturing applications. I will use the model to describe the evolution of the height profile, contact radius, and hence the volume of the droplet from its initial configuration until total evaporation. In particular, I will show how the evolution of the droplet is qualitatively dependent on the cross-sectional profile of the well. I will then compare the theoretical predictions of the model with detailed experimental results for the evaporation of droplets in cylindrical wells of various sizes, and show that the theory and experiment (and in particular, the critical times at which the droplet first touches down and at which total evaporation occurs) are in excellent agreement.

11:00am - 11:30am

**Minisymposium 14B: Mathematical Modelling of Lithium-Ion Batteries**

**Chair:** Matthew Hunt
**Session Chair:** Jamie Michael Foster

**Multiscale modeling of lithium batteries**

**Jeta Molla, Markus Schmuck**

Heriot-Watt University, United Kingdom

We consider basic and easily extendible transport formulations for lithium batteries consisting of an anode (Li-foil), a separator (polymer electrolyte), and a composite cathode (composed of electrolyte and intercalation particles). Our mathematical investigations show the following novel features: (i) complete and very basic description of mixed transport processes relying on a neutral, binary symmetric electrolyte resulting in a non-standard Poisson equation for the electric potential together with interstitial diffusion approximated by classical diffusion; (ii) upscaled and basic composite cathode equations allowing to take geometric and material features of electrodes into account; (iii) the derived effective macroscopic model can be numerically solved with well-known numerical strategies for homogeneous domains and hence does not require to solve a high-dimensional numerical problem or to depend on a computationally involved multiscale discretisation strategies where highly heterogeneous and realistic, nonlinear, and reactive boundary conditions are still unexplored. We believe that the here proposed basic and easily extendible formulations will serve as a basic and simple setup towards a systematic theoretical and experimental understanding of complex electrochemical systems and their optimization, e.g. Li-batteries.

11:30am - 12:00pm

**Electrode heterogeneity in lithium ion batteries**

**Jon Chapman, Toby Kirk, Colin Please**

University of Oxford, United Kingdom

The standard porous electrode theory of lithium ion batteries involves solving a lithium intercalation problem (usually a diffusion problem) on a representative electrode particle at each point in the macroscopic (homogenised) model. Usually the representative particles are taken to be spheres all the same size.

Here we consider the implications of a distribution of particle size on such models, that is, we have a representative distribution of particles rather than a single particle at each point.

12:00pm - 12:30pm

**On the (dis)charge of LiFePO4-based Li-ion battery electrodes**

**Michael Jack Castle**, Rahifa Ranom, Giles Richardson, Jamie Michael Foster

1University of Portsmouth, United Kingdom; 2Universiti Teknikal Malaysia Melaka, Malaysia; 3University of Southampton, United Kingdom
We present a model for the (dis)charge of a Li-ion battery cathode comprised of LiFePO4 nanoparticles, based on porous electrode theory introduced by Newman and co-workers in the mid 90’s. This modelling approach describes the electrochemical processes inside a Li-ion electrode via a multiscale system of PDEs for the Li concentrations, electric potentials, and current densities inside the device. We show that for LiFePO4 electrodes, which have an unusually flat open circuit potential, there is an asymptotic solution to the model which exhibits sharp moving discharge fronts (one side of which the electrode material is fully charged and on the other it is fully discharged). We demonstrate favourable agreement between the asymptotic solution and a wholly numerical solution. Finally, we make some comments on how the solutions suggest strategies for designing LiFePO4 electrodes which can offer enhanced performance.

11:00am - 12:30pm Contributed Talks 17: Granular media Session Chair: Gleb Zhelezov

11:00am - 11:20am

Modelling granular media using Dynamical Density Functional Theory

Timothy David Hurst¹, Ben Goddard¹, Raffaella Ocone²
¹University of Edinburgh, United Kingdom; ²Heriot-Watt University, United Kingdom

Systems of granular media play several important roles in industry and the natural world. Their dynamics are very complicated, as microscopic interactions between particles can have a large effect on the entire system. This also presents a difficulty when trying to model a system of granular media: even state of the art computational power cannot handle a large enough number of particles to fully simulate a system of industrial scale, and existing continuum models can neglect important particle interactions that take place, which can make their flow predictions inaccurate. Recently, dynamical density functional theory (DDFT) has proved successful in modelling colloidal fluids, such as paint or milk. DDFT incorporates interparticle interactions and volume exclusion at a mesoscopic level, using the well-studied Helmholz free energy functional. They can be fine-tuned by deriving empirical forms of parameters from particle simulations with small numbers of particles. We present a new DDFT that is suitable for granular media. A model is constructed which includes volume exclusion effects and other interparticle interactions via the free energy functional, but also includes effects from inelastic collisions using a collision operator. We simulate small systems of inelastic hard particles using event driven particle dynamics (EDPD), and use statistics from these simulations to construct parameters that are not analytically tractable, for example the radial correlation function. These parameters are then used in example DDFT simulations. The results are promising, and along the way, several important and fundamental questions relating to granular media during the derivation.

11:20am - 11:40am

Dynamic Density Functional Theory: Well-Posedness, Global Asymptotic Stability

Ben Goddard¹, Rory Mills-Williams¹, Grigoris Pavliotis²
¹University of Edinburgh; ²Imperial College London

We establish, for the first time, the global well-posedness of overdamped dynamic density functional theory (DDFT): the nonlinear, nonlocal integro-partial differential equation used in many statistical mechanical models of colloidal flow. Analogous equations arise in many areas, including the McKean-Vlasov equation [1], pattern formation, flocking of birds, and cell proliferation. The results hold for more physically realistic boundary conditions than those previously considered. This allows application to a variety of physical and biological systems including non-local reaction-diffusion equations, Ohmic heating and opinion dynamics. The results are achieved by studying the bounded perturbation of the local differential part of the linearised operator. We show the spectral properties of the full non-local operator can differ considerably from those with simpler, e.g. periodic, boundary conditions. We showcase our results by using the numerical methods available in the pseudo-spectral collocation scheme 2DChebClass [2].

[2] 2DChebClass - https://datashare.is.ed.ac.uk/handle/10283/2647

11:40am - 12:00pm

Diffusion processes at nanoscale

Claudia Fanelli¹,²,³
¹Centre de Recerca Matemàtica, Barcelona, Spain; ²Universitat Politècnica de Catalunya, Barcelona, Spain; ³Barcelona Graduate School of Mathematics, Barcelona, Spain.

Nanoparticles are units of matter with dimensions between 1 and 100 nanometers (nm) that have gained a lot of interest during the last decades, due to their wide variety of applications in biomedicine, environmental-related problems, electronics and catalysis. It is well-known that many properties of nanoparticles, such as luminescence, photostability, optical radiation efficiencies and electric properties among others, are size dependent. Hence, the ability to create nanoparticles of a specific size is crucial.

A model for the process of synthesizing nanoparticles of the required size from a liquid solution is shown. Initially, I will describe a single particle model that accounts for a diffusion equation for the concentration of the solution and a mass balance (equivalent to a Stefan condition) for the evolving particle radius [1]. The model is then extended to a system of N particles and numerical solutions for the time-dependent average particle radius compared to experimental data are shown [2].

Once provided a mathematical description of the NP growth process and guidelines for efficient growth strategies, I will show a specific practical application of NPs, namely targeted drug delivery [3]. The ultimate goal will be to determine strategies to maximise drug delivery to a specific site. The physical situation
modelled involves the motion of a non-Newtonian nanofluid subject to an external magnetic field and an advection-diffusion equation for the concentration of nanoparticles in the fluid.

12:00pm - 12:20pm
Application of the compressible I-dependent rheology to chute and shear flow instabilities

James S. Fannon¹, Iain R. Moyle², Andrew C. Fowler¹,³
¹MACSI, Department of Mathematics and Statistics, University of Limerick, Limerick, Ireland; ²Department of Mathematics and Statistics, York University, Toronto, Canada; ³OCIAM, University of Oxford, Oxford, UK

The flow of granular material constitutes an everyday occurrence which plays a fundamental role in both industry and the natural world. The pharmaceutical, food manufacturing, and mining sectors rely heavily on the handling and processing of granular material on a daily basis, while a comprehensive understanding of the behaviour of such material is essential for the mitigation of risks posed by destructive geophysical flows, such as avalanches. Granular material is found to demonstrate three different types of flow behaviour, namely solid, liquid, and gas-like behaviour. This liquid-like flow is the most frequently encountered in practical applications of interest, and the continuum modelling of this regime has attracted significant interest in the literature.

In this talk we present a recently proposed compressible hydrodynamic model for dense granular flow and test its veracity against flow instabilities observed in two different geometries. We perform a full linear stability analysis of the model equations and compare its predictions against experimental data for inclined plane flow and discrete element simulations of plane shear flow. In the case of the former, a normal mode analysis yields a generalised eigenvalue problem which is solved using a Chebyshev collocation method. We find that the compressible model can quantitatively capture the experimental data. In the latter case, we solve the linear stability problem analytically and demonstrate that the model also accounts for the observed instability.

12:30pm - 1:30pm
Lunch
Foyer, Level 1

1:30pm - 2:30pm
Plenary 7: The QJMAM Fund Lecture
Session Chair: Christopher Budd

The mathematical theory of geophysical flow models - challenges and some results
Beatrice Pelloni
Heriot-Watt University, United Kingdom

The mathematical and numerical analysis of models for atmospheric flows is still a formidable mathematical challenge. The semi-geostrophic equations are a particular system of partial differential equations, widely used in the modelling of large-scale atmospheric flows. In this talk I will review the mathematical ideas and results that have enabled spectacular progress in the past 25 years, as well as discuss the many problems that are still open.

2:30pm - 3:00pm
Plenary session: Prize presentations
CB 1.10

3:00pm - 3:30pm
Coffee and departures
Foyer, Level 1