BAMC 2022

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Contributed talk abstracts

Brainstem Oscillators and Bifurcations: Understanding How Circadian Clocks Communicate

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Analysis of bioluminescent rhythms recorded in the mouse brainstem reveals a characteristic phase relationship between three distinct circadian oscillators: the area postrema (AP), the nucleus of the solitary tract (NTS) and the ependymal cells surrounding the 4th ventricle (4Vep). The data strongly suggests a consistent behaviour in which AP peaks first, followed shortly by the NTS, with the 4Vep peaking 8-9 hours later. I will talk about how we've used phase-coupled oscillator theory to discover a minimal model that is consistent with the data. Using phase-plane and bifurcation analyses, it is discovered that coupling of the AP with the NTS and 4Vep is necessary and that a phase delay is required in the AP-NTS coupling in order to capture the phase relationship between the peaking orders. The model is consistent with findings from experiments in which mechanical and chemical treatments had been applied. Keywords: mathematical biology; neuroscience; bifurcations; kuramoto; phase model; oscillators; synchronization

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Towards a multiphase model of vascular network formation in a hydrogel

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Introduction: Vascularisation of engineered tissues is essential to ensure sufficient nutrient supply once implanted in vivo [1]. Prevascularisation of the engineered tissue by seeding with endothelial cells (ECs), which can form capillary-like structures in vitro and anastomose with host vasculature upon implantation, is a promising method to accelerate vascularisation [1]. Based on a balance of chemical and mechanical cues, the mechanisms involved in EC network formation can be explored computationally with use of mechanistic mathematical models [2]. Here, we adopt a multiphase model framework to investigate the impact of ambient and intercellular oxygen concentration on the formation of EC networks in vitro. We focus on the production of vascular endothelial growth factor (VEGF), produced by ECs under low oxygen that guides EC migration and promotes vascular network formation [1].

Methods and Results: A multiphase model consisting of a set of 8 coupled PDEs is used to describe the temporal and spatial development of the endothelial cell distribution, oxygen and VEGF concentrations within a 3D hydrogel. Crucially, the flexible model framework integrates global features such as construct geometry and environmental conditions, with intercellular mechanisms that lead to network formation [2, 3]. Mechanisms include autologous chemotaxis, oxygen-dependent VEGF production, and cell-matrix interactions mediated by cell traction and matrix stiffness.

A 2D axisymmetric model is implemented computationally in Python, allowing utilisation of computational techniques including sensitivity analysis and parameter optimisation, to identify parameter ranges under which different multi-cellular structures emerge. A methodical approach is taken to discover a suitable function form for cell- and oxygen- dependent VEGF production, based on a combination of simulation, existing data, and data from tailored in vitro experiments. We validate our computational model against in vitro data for a range of ambient oxygen levels, including continuous intercellular oxygen levels and total amount of VEGF in culture media.

Discussion: This flexible computational model allows investigation of the role played by a range of experimental conditions in vascular network formation within a 3D construct, including hypoxia, which has increasingly recognised significance [1, 4]. It is hoped that simulation predictions, validated by further data, will aid and inform the culture methods of prevascularised engineered tissues for clinical use.

References: 1. Rouwkema J, Khademhosseini A. Trends in Biotechnology 2016; 34(9):733-745. 2. Scianna M et al. Journal of Theoretical Biology 2013; 333:174-209. 3. Lemon G et al. Journal of Mathematical Biology 2006; 52(5):571-594. 4. Hsu, H et al. Small 2021; 2006091.

Keywords: mathematical biology; computational methods; multiphase model; cell migration; chemotaxis; pattern formation; parameterisation

Bifurcation Analysis for a System of Rational Difference Equations

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In this paper, we study dynamic behavior for a system of rational difference equations. We derive analytical conditions for stability of the fixed point(s) of the system. Moreover, we investigate the one and two-parameter bifurcations of the system. For all bifurcations, the topological normal forms are computed. To confirm the theoretical results, we performed a numerical bifurcation analysis by using the MATLAB package MatContM, which performs based on the numerical continuation method.
Keywords: Difference equations; bifurcations; topological normal forms; Lyapunov exponent; MatContM.

Basic physical mechanisms responsible for three-dimensional wake transition

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We consider the general problem of 3D vortices appearance in incompressible viscous fluid flows, which admit 2D solutions, using the time-periodic flow in the wake behind a circular cylinder as an example. We show that in this flow, the balance of the following two factors determines the overall flow stability: the repeating growth of perturbations in each forming vortex (which can be observed long before the threshold of modal 3D instability) and the feedback mechanism which creates the perturbations of certain "initial amplitude" in a new vortex upstream. The basic mechanisms that govern the initial development of 3D vortex structures are vortex line stretching by the base flow strain field, transfer of the base flow vorticity due to tilting, and viscous diffusion. We analyse the action of these mechanisms for the (quasi-)periodic solutions, which describe various patterns of the 3D wake and are obtained using the Floquet theory at a wide range of the Reynolds numbers and spanwise wavelengths. In addition, we reveal the key regions of perturbation kinetic energy generation and the mechanisms of its redistribution.

The research was supported by the Royal Society Newton International Fellowship (NIF R1 201343). The authors would like to acknowledge the assistance given by Research IT, and the use of the HPC Pool funded by the Research Lifecycle Programme at the University of Manchester. Keywords: hydrodynamic stability, bluff body flows, wakes, computational fluid dynamics

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Modelling elastic wave band-limited uniform diffusers

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We present a modelling approach to design elastic wave diffusers, for both compression and shear waves. The technique for generating randomly characterised surfaces with a prescribed mean reflection intensity has previously been implemented for polarised electromagnetic waves [1]. Here, we use a similar approach for the more complicated elastic vector problem, with an application to one-dimensional rough surfaces. Different types of diffusers have been investigated, including band-limited uniform and Lambertian diffusers, using a stochastic approach to generate randomly rough surfaces with the prescribed mean angular intensity distribution. For compression wave incidence, the theory allows for the generation of surfaces with a prescribed intensity distribution for both the reflected compression wave mode (P-P) as well as the mode-converted vertically polarized shear wave (P-SV). We envisage developing the elastic diffusers for two dimensional rough surfaces, including the investigation of more exotic effects involving enhanced backscattering and transmission problems.

References: [1] Leskova, T.A., Maradudin, A.A, Novikov, I.V., Shchegrov, A.V. & Mendez, E.R. " Design of one-dimensional band-limited uniform diffusers of light", Applied Physics Letter 73(14). (1998)

Keywords: Elastic wave scattering; stochastic processes; mathematical design; non-destructive testing

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A mathematical model of macrophage phenotype switching and its role in the resolution of inflammation

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Inflammation is a natural response of the immune system to harmful stimuli, such as pathogens, toxic compounds, and damaged cells. The primary function of inflammation is to protect living tissue by eliminating and removing injurious stimuli and restoring tissue homeostasis. Therefore, inflammation is an essential part of the body's natural defence mechanism. The aetiologies of inflammation are varied and may be non-infectious or infectious factors. Thus, symptoms of inflammation vary depending on the cause of the injury or the site of injury. However, symptoms may include pain, fatigue, and fever. There are two main types of inflammation, each varying in intensity and duration: acute and chronic. We can think of acute inflammation as the immune system's early biological response to injury that is generally beneficial to the host. By contrast, chronic inflammation is the persistent harmful type that can lead to significant organ dysfunction. Inflammation is associated with a wide range of chronic inflammatory diseases, including, but not limited to, heart disease, numerous autoimmune diseases, type 2 diabetes, cancer, metabolic disorders, arthritis. Thus, chronic inflammatory diseases are among the most common cause of death in the world.

This study aims to understand the key role of macrophages in inflammation, focusing on the resolution of inflammation by constructing a time-dependent mathematical model, which will be formulated as systems of ordinary differential equations (ODEs). Our mathematical model focuses on the interactions between two distinct populations of macrophages, such as M1 (classically activated macrophages) and M2 (alternatively activated macrophages) and pro- and anti-inflammatory mediators. Our model provides useful insights into the essential role of the phenotype of macrophages in the resolution of inflammation; we investigate the different qualitative behaviours presented by our model and discuss them in terms of the inflammatory response and its potential results. We also use bifurcation diagrams to investigate how variation in the system's key parameters influences the switch between chronic and resolved (healthy) outcomes. Keywords: Mathematical Biology, Inflammation, Macrophage, Differential Equations

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Parallel computations of superfluid vortex systems

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Superfluids are quantum fluids that flow without dissipation and present a new turbulence species called superfluid turbulence. Superfluid turbulence (or Quantum Turbulence) is essentially a tangle of interactive vortex filaments of quantised circulation. In order to understand superfluid turbulence with very dense vortex tangles, we have developed a parallel vortex dynamics code that computes the Biot-Savart velocities and allows us to probe the physics of very dense vortex tangles, as well as coupling the latter with normal fluids described by the Navier-Stokes equations. This talk is confined to the pure superfluid case. Our code employs the message passing interface parallel computation model and is implemented in a shared memory machine with 116 threads. I present calculations with reconnecting and interacting bundles of superfluid vortices that resemble classical filaments. These two configurations involve superfluid vortex bundles in colliding and Hopf link initial settings. I discuss vortex configurations and reconnections including key physics conclusions. Keywords: Superfluids, Superfluid Vortex Tangles, Superfluid Vortex Dynamics, Superfluid Turbulence, Biot-Savart velocity, Parallel Computations

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Mathematical Modeling and Simulation of Nanofluid Flows

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Conventional heat-transfer fluids like water, oil, and ethylene glycol used in cooling systems have limits to their effectiveness due to their low thermal conductivity. Using millimeter and micrometer-sized solid particle suspensions in these fluids leads to the problems of sedimentation and corrosion, especially in the miniaturized devices where the cooling fluids are required to circulate in narrow spaces. Nanofluids have been investigated for their potential to be an alternative to conventional fluids in heat-transfer systems. There has been considerable research to study the slip mechanisms between suspended nanoparticles and the base fluid that lead to the relative velocity between two phases and promote heat exchange. Brownian diffusion and Thermophoresis are observed to be two significant slip mechanisms that increase the heat transfer rate, although some other studies have found a limited influence of Brownian diffusion on the heat transfer. This study was undertaken to investigate the heat transfer characteristics of a nanofluid using Al_2O_3 nanoparticles suspended in water as the base fluid under natural convection in a rectangular enclosure. The enclosed nanofluid is subject to a temperature gradient that causes laminar convection to be established. The thermal conductivity of the nanofluid was examined by running MATLAB simulations. Four different models were classified based on different formulae for dynamic viscosity and thermal conductivity. The numeric simulation was performed using MATLAB software using Rayleigh numbers ranging from 10^4 to 10^6. Streamline contours were computed and the results were compared with similar published studies. The results were found to agree with the published research. Keywords: Nanofluid flow, Convective heat transfer, Thermal conductivity, Dynamic viscosity

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Asymptotic Analysis Of The Vitamin C Clock Reaction: The Effect of Hydrogen Peroxide Concentration On The Effective Kinetic Law

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The study of chemical kinetics has been carried out for over 100 years. The term "clock reaction" was studied for the first time by Landolt in the 1880s. Chemical clock reactions are identified by a predictable induction period followed by a rapid change 'switchover', allowing the clock chemical concentration to rise. The purpose of this research is to use mathematical modelling and analysis to gain insights into the chemical clock reaction and associated vitamin C and hydrogen peroxide. A new model, in the form of four nonlinear differential equations, is designed to track the hydrogen peroxide concentration. The model is studied through asymptotic analysis

and computational investigation. Recent mathematical modelling has hydrogen peroxide concentration in great excess compared to the other reactants, resulting in the oxidation reaction producing the clock chemical iodine from the reaction of iodide with hydrogen peroxide is quadratic in iodide concentration. This research will address the question of whether the clock chemical reaction converting iodide to iodine should be quadratic in iodide or linear, and the potential role of hydrogen peroxide concentration. The difference in forward and backward reaction rates results in a small parameter upon which a time-dependent matched asymptotic expansion can be performed. Asymptotic approximations in the appropriate time regions agree closely with the numerical solutions. The analysis also produces an approximate formula for the dependence of switchover time on the initial concentration of the reactants. We demonstrate how the order of the ratio of hydrogen peroxide to iodide determines when linear kinetics apply and when quadratic kinetics apply. Keywords: Mathematical modelling, clock reaction, vitamin C, hydrogen peroxide, asymptotic analysis.

Fundamental modes of swimming correspond to fundamental modes of shape: Engineering I-, U-, and S-shaped swimmers

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Artificial microswimmers have the potential to accomplish complicated tasks such as drug delivery, cargo transport, and automated surgery at the microscale. These microbots employ a number of propulsion mechanisms and different materials to function in the Stokes regime. Bubble propulsion, as an example of such mechanisms, uses chemical reactions between swimmer's surface and environment to fuel locomotion. Hydrogels are a promising material for the manufacture of bubble-propelled microbots due to their biocompatible properties, versatility, and possible shape transformations. In this study, 3 different bubble-driven microbots, manufactured via stop-flow lithography (SFL), are combined with various configurations of active catalytic and passive regions. I-, U-, and S-shaped swimmers correspond to the first 3 bending modes of an elastic filament. We investigate the motion of swimmers and bubble-growth dynamics on active regions. The dynamics of the bubbles can be categorised into 2 main stages, growth and collapse, which result in steady propulsion and sudden impulse by jet, respectively. Our mathematical model and image analysis suggest an approximately constant molar flux of reactant product gas into the growing bubbles. Our model also reveals a decay in maximum bubble radius and increasing growth time over many cycles, suggesting degradation of the enzyme in the active portion of the hydrogel. Finally, the mechanism of bubble collapse is examined, and the Blake critical radius of collapse is approximated. In the future, the implementation of bubble-propelled shape transforming hydrogels can pave the way for performing a number of complex tasks at the microscale.
Keywords: Artificial microswimmers, active matter, bubble dynamics

Selection mechanisms and complex singularities in the rising bubble problem

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The precise characterisation of the set of steady-state solutions for a rising bubble in a tube remains an open problem. Here, we consider a two-dimensional bubble which rises, under the influence of gravity and at constant velocity, in a tube filled with an ideal fluid. When surface tension is included, it is known that the velocity of the bubble must be selected from a countably infinite set of possible values. This is similar to the selection mechanism in the classic Saffman-Taylor viscous fingering problem but the introduction of gravity complicates the analysis of the rising bubble. In this talk, we discuss the surprising complexity that characterises the complex analytic structure of the zero surface-tension case, and also the challenges of resolving this selection mechanism in the small surface tension limit. Keywords: asymptotic analysis, fluid mechanics, potential flows

In silico model for cell therapy in acute liver injury

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Successful clinical translation of cell therapies requires robust preclinical approaches to assess their safety, toxicity and efficacy. We focus on liver cell therapies, and combine *in silico* and *in vivo* approaches to determine how interactions between the donor cells and the injury site impact their ability to engraft and restore liver function.

In vivo, we induce acute liver injury via drug administration, which in turn results in host liver cell senescence, impacting their ability to proliferate and function. The injected donor cells transit through the vasculature until they reach the small blood vessels of the liver. They then extravasate across the blood vessel wall reaching the injury site, where they will either be removed by the macrophages or attach to the extracellular matrix (ECM) and engraft. The goal is to maximise the number of cells that engraft to promote regeneration of the injured liver.

We develop and solve an ordinary differential equation (ODE) model capturing the interactions between the donor cells and the senescent host environment. The dependent variables are senescent, macrophages, endothelial, and myofibroblast cell populations and ECM concentration (all species variables are relative to baseline). The ODEs are derived via a conservation of mass argument for each species (cell population or concentration), accounting for, e.g., proliferation, death/removal, and source and sinks of each cell type/concentration due to cell-cell or cell-ECM interactions e.g. the removal of donor cells by macrophages is captured via sink term. The system is driven by the induced senescence level, which results in an initial increase in species populations/concentration. We determine the steady states and their stability to small amplitude perturbations, and hence identify regions of parameter space where a unique stable solution exists corresponding to baseline values. The time-dependent ODEs are solved numerically in MATLAB. Depending on the level of initial senescence and the system parameters, we show that the system will either resolve (species variables return to baseline values) or results in inflammation (species variables do not return to homeostasis levels).

We investigate the effect the initial senescence level has on the ability of the system to resolve in the absence of donor cells. We then introduce a population of donor cells, investigating their ability to aid resolution via their engraftment into the liver. Parameters such as the initial donor cell population and the time of injection relative to the time of induced senescence are examined. We validate these results with experimental observations with and without the addition of the donor cells.

Comparison of these complementary data sets can provide insights into what interactions are dominant for the successful engraftment. These insights can be used to guide and optimise novel cell therapy protocols.

Keywords: mathematical biology; modelling; cell therapy; cells interactions

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Internally Heated Convection at Infinite Prandtl

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Bounding, a priori, the heat transport in convection, with respect to the Rayleigh number has been an important and still unresolved question in the fluids and applied maths communities since the 1960s. The standard, boundary driven convection (Rayleigh-Bènard) has and continues to be extensively studied, experimentally, numerically, and analytically. However, in nature, we find many physical systems exhibiting convection driven, at least partially, by internal sources of heat. We formulate rigorous bounds by use of the background method, whereby one splits a field into a background and perturbation component, each of which satisfying different conditions. Our investigation is in the limit of Infinite Prandtl numbers for uniform internally heated convection and we prove for the first-time upper bounds on the mean convective heat transport. These can be interpreted as bounds on the Nusselt number, in analogy with Rayleigh-Bènard, or as the heat flux out of the boundaries, to quantify the asymmetry induced internally heated convection. Critical to our proof is a minimum principle for the temperature, piecewise logarithmic choices for a background temperature profile and Hardy-Rellich type integral estimates.

Keywords: geophysical fluid dynamics, variational methods, bounding

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High-order adaptive time-stepping methods for nonlinear fractional DEs

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We have developed fully discrete, high-order, adaptive time-stepping methods for fractional differential equations. The methods are based on the kernel compression scheme for the approximation of the history term and on the integral deferred correction method (IDC) for the approximation of the local term. The analysis shows that the IDC method increases the order of the local approximation each correction iteration. Numerical examples are provided to validate the theoretical results and to demonstrate the efficiency of the proposed methods. The results demonstrate the capability to yield high order accuracy and the ability of the error indicators to control the error, detect changes in the solution, and adapt the step size accordingly. Keywords: fractional differential equations; numerical analysis; integral deferred correction method; kernel compression scheme

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Mathematical modelling of the effect of climate variations on cocoa production

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University of Bath

Chris Budd, University of Bath

Cocoa is an important crop that is predominantly grown in the western part of Africa. However, there have been fluctuation and declining trend in production and many factors have been identified to be responsible. A significant factor is the effect of climate variation and this result in low farm-level yield. To understand the contribution of climate variability on the farm level yield, we construct and analyse a time delayed model for the effect of rainfall on productions. This work uses a system of delay differential equations to model to the crop transition from the flowering stage to pod formation and harvesting. We introduce a forcing function into the model to account for the seasonal rainfall and then conduct a sensitivity analysis to understand the effect of model parameters. This leads to a novel nonlinear ODE for the flowering with periodically varying coefficients. This is couple to a DDE for the pod formation and harvesting. Finally, we perform an analysis of all parts of the system and this shows that it has a 6 month periodic solution which connect to the seasonal rainfall for different parameter ranges. Keywords: Asymptotic analysis, Cocoa production, Climate variation, Delay differential equation, Periodic solution and Rainfall function

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Bifurcation analysis of bi-stable stochastic nonlinear dynamical systems with near-periodic solutions

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David A.W. Barton, Henrik Sykora** – *University of Bristol, **Heriot-Watt University*

Hopf bifurcations are frequently used to characterise self-excited vibrations in many engineering applications such as machining, tyre- and vehicle dynamics, or aeroelastic flutter. The structure of the limit cycles associated with Hopf bifurcations in deterministic nonlinear dynamical systems is well-understood and thoroughly researched. The technique of Control-based Continuation (CBC) enables bifurcation analysis in physical experiments where the exact governing equations are not available. Experiments however are often subject to considerable process noise and, as such, analysing them in a deterministic framework may not entirely capture their true behaviour. A further challenge with the CBC method is that it assumes that a control-target corresponding to non-invasive control (i.e., when the steady-state control input to the system is zero) can be found, which is generally not the case in systems with random excitation. This raises the question on the limitations of the deterministic models of experiments and that in what extent is it possible to extract the underlying deterministic dynamics from a noise-polluted experiment. This study investigates the relationship between the near-periodic solutions in a stochastic nonlinear system with and without CBC and the limit-cycles of the underlying deterministic system. We analyse the Hopf normal form with quintic nonlinearity and random excitation focusing the case when a bi-stable parameter domain, where the equivalent deterministic system has a co-existing stable equilibrium and a limit cycle appears. We obtain the time-evolution of the probability density function (PDF) of the stochastic system. Then, the near-periodic solutions are characterised based on the steady-state PDF which is a deterministic feature of the system. We demonstrate that random excitation results in stable near-periodic oscillations around the stable equilibrium of the deterministic system. With CBC, the corresponding solution branch is found to be connected to the branch equivalent to the unstable limit cycles in the deterministic system. Thus, the original Hopf bifurcation becomes saddle-node-like. The role of the unstable limit cycles is also interesting in the stochastic system. Even though it is possible to stabilise the system around them with control, they never appear directly in the open-loop system. Still, the deterministic case suggests that they can be used as an indicator of the boundary between the domains of attractions of the two attractors in the bi-stable domain. Nevertheless, our analysis shows that the identified characteristic vibration amplitudes of the stochastic system are different from the deterministic case.

Keywords: stochastic dynamical systems, nonlinear dynamics, bifurcation analysis, continuation

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Modelling Regenerative Angiogenesis in Peripheral Nerve Repair

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Around 5% of traumas result in Peripheral Nerve Injuries (PNIs), affecting more than 1M people per year in Europe and the USA. Paralysis and loss of sensation are hallmarks of severe PNIs, which can lead to lifelong pain and disability for patients. Large-gap PNIs cannot repair unaided and generally require a surgical intervention by mean of an autograft. This induces donor site morbidity and tissue availability is limited. Engineered Neural Tissue (EngNT) constructs are being developed to address the challenges raised by autografts. They are cylindrical anisotropic cellular hydrogels that mimic nerve tissue and provide a supportive microenvironment to accelerate regeneration, whilst also enabling spatial seeding of therapeutic cells and other regenerative factors. In particular, these cells can secrete vascular growth factors that act as chemical cues for the formation of a new microvasculature, the latter being a key player in nerve regeneration. A central challenge is then to evaluate the consequences of using a given therapeutic cell type, density or spatial distribution on revascularisation and long-term regeneration. To address this, we develop a mechanistic description of the vascular regeneration process. We develop a system of effective continuous, coupled, non-linear, diffusion-reaction equations that we parameterise using dedicated in vitro experiments. Doing so allows us to describe the interplay between the therapeutic cells and their microenvironment, including cell proliferation, nutrient consumption, and growth factor secretion. We then overlay this continuous description with a pore network model obtained using upscaling methods (Volume Averaging, Multiscale Asymptotics) that account for vessel growth, blood flow and molecular exchanges between the vasculature and the surrounding microenvironment. Coupling these two models allows us to reproduce the complex spatio-temporal dynamics between blood flow, angiogenic processes, oxygen delivery, growth factors and seeded cell population during nerve repair. Simulations are performed for different therapeutic cell types and for a range of cell-seeding densities and spatial distributions to explore the impact on angiogenesis and cell survival. They indicate that seeding cells beyond a given threshold appears to be detrimental for long-term cell survival and vascular regeneration but that seeding them preferentially close to the nerve stumps can help sustain gradients of growth factors in the nerve repair construct. This modelling approach therefore allows us to explore efficiently a wide variety of scenarios and identify new cell seeding strategies that may accelerate revascularisation of a repair construct and improve cell survival to be taken forward to in vivo experimental testing.

Keywords: Angiogenesis, Multiscale, Multiphysics, Biomaterial

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Curious dynamics of a golf ball bounce

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Stanislaw Biber, Alan Champneys, Robert Szalai

The bounce of a ball in sports such as tennis, cricket or football has been studied extensively with many experimental data available to support the analysis. The common denominator for these models is an impact of a compliant ball off a rigid ground. A bounce of a golf ball is a very different problem though, where the analysis focuses on the impact of a rigid body off a compliant surface. Previous studies of this problem have been largely limited by the lack of experimental data.

In our talk we present our approaches at modelling the bounce of a golf ball where we try to match the physical intuition with experimental data. We extend previous work by creating large experimental campaigns. In the modelling we carefully distinguish the slipping and rolling (sliding) scenarios and we approach the problem with a wide spectrum of initial conditions in mind. The distinction between slipping and rolling cases introduces a discontinuity in the dynamics, as the friction forces are only known for the slipping scenario. This means that the dynamics for rolling happen in the region of discontinuity and must be carefully defined – such systems are known in the literature as Filippov systems.

We analyse a generic non-linear and non-smooth dynamical system which models the bounce under the assumption of Coulomb friction force. In this we look at the peculiarity which comes from the fact that the condition for the lift off of the ball consists the two fold bifurcation point – a point where the ball undergoes two different discontinuous changes in the dynamics. It can be shown that in such non-smooth system it is only possible for the ball to exit the bounce slipping (and never rolling). In the final part of our talk we will link our analytical results to the experimental observations. We will further discuss the challenges and solutions relating to the problems of matching experimental data to non-smooth dynamical systems. Keywords: Applications of dynamical systems, Non-smooth dynamics, Filippov systems,

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Towards a model-free bifurcation analysis of autonomous slow-fast systems

Mark Blyth

University of Bristol

Mark Blyth, University of Bristol. Lucia Marucci, University of Bristol. Krasimira Tsaneva-Atanasova, University of Exeter, Bulgarian Academy of Sciences. Ludovic Renson, Imperial College London.

Mathematical modelling provides a rigorous approach to communicating one's interpretations of the natural world. Much work has gone into developing a sophisticated arsenal of computational tools for studying models; nevertheless, these models are not absolute truths so much as mathematical metaphors, and the results of any analyses are only as representative as the models they were obtained from. An intriguing

alternative would be to skip the modelling step entirely, and apply standard analysis methods directly to a real-world system. Control-based continuation is a recently developed method for achieving this, and uses feedback control to define a model-free zero problem on a physical system. The zero-problem can then be combined with numerical continuation methods, for example to perform a model-free bifurcation analysis. Here I will introduce control-based continuation, and highlight some of the challenges that arise when using it to study autonomous slow-fast systems. The zero-problem is constructed using a controlled system, and behaves as a noisy and nonlinear black-box operator. Particular attention is paid to discretisation methods for these operators, as well as to the choice of phase conditions for constructing a well-posed continuation problem. Simulated results are shown with a neuronal system, and some future challenges are considered. Keywords: Experimental nonlinear dynamics, neuronal dynamics, numerical continuation, control-based continuation

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Towards a model of a deformable aerofoil

Mark Blyth

University of East Anglia

Adam Yorkston (UEA), Emilian Parau (UEA)

Aerofoils that include flexible components are designed to enhance aerodynamic capability and to promote fuel efficiency under a range of different flight conditions. Some small, unmanned aerial vehicles (UAVs) use entirely collapsible, elastic wings to maximise portability. In this talk we work toward a model of a deformable aerofoil by studying the behaviour of a thin-walled elastic cell in a uniform stream. We use a conformal mapping approach to determine the cell shape and the ambient flow simultaneously. Our initial analysis of a light cell in an oncoming flow can be viewed as a generalisation of Flaherty et al.'s 1972 work on the buckling of an elastic cell under a constant transmural pressure difference. Introducing cell mass and circulation/lift, we study equilibrium shapes at different flow speeds and for different transmural pressure jumps. A fixed-angle corner at the trailing edge is introduced by way of a Karman-Trefftz conformal mapping, and an internal strut is included, to more accurately mimic the shape and aerodynamic properties of a traditional, rigid aerofoil. DNS simulations are carried out to assess the performance of the equilibrium aerofoil shapes in a real flow. Keywords: Fluid-structure interaction, aerodynamics

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Mathematical modelling of poroelastic tissue engineering scaffolds within bioreactors

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To engineer functional tissue, we need to provide appropriate biomechanical and biochemical cues to promote cell proliferation and differentiation. Mathematical modelling aims to provide a mechanistic understanding of cell growth, fluid flow and nutrient and waste transport in these systems to inform experimental design. Inspired by human vasculature, our work focuses on modelling electrospun hollow fibre membranes for use in tissue engineering bioreactors.

Experimental collaborators at the University of Oxford have developed a hollow fibre membrane scaffold that mimics the deformability and distensibility of human vasculature. The ends of these fibres are fixed in a bioreactor chamber, and cells are seeded to the inner or outer surface. Fluid flow is used to enhance nutrient and growth factor delivery through the fibre lumen, and waste products can also be removed through an additional flow outside of the fibres.

We develop an axisymmetric fluid-structure interaction model of steady Stokes flow in and around a linear poroelastic membrane fibre clamped at its axial ends. Exploiting the small aspect ratio and the large stiffness of the membrane fibre relative to typical fluid pressures, we use asymptotics to derive a coupled system of linear second-order PDEs and ODEs describing membrane displacement and fluid pressure respectively. With this, we solve for fluid flow through the lumen, membrane and extra-capillary space. At leading order, the fluid flow problem reduces to Darcy flow through a rigid porous material, and membrane displacement is driven by the membrane fluid pore pressure. We extend this model to consider spatially-dependent membrane permeability and investigate how compressibility, membrane thickness, inlet fluid pressures and permeability can be controlled to optimise fluid flow to cells seeded along the length of the fibre surface. In addition to providing mechanistic insights into the mechanical environment of the cells, these models can be used to inform future scaffold design. Keywords: Fluid Mechanics, Poroelasticity, Asymptotic Analysis, Tissue Engineering

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Statistical analysis of trade risk, failure, and extreme event propagation in the global economy using multi-level networks

Malvina Bozhidarova

University of Nottingham

Global financial stability has become one of the key concerns of economic policy-makers and decision-makers due to the increasing frequency, magnitude and international scope of financial crises. Interconnectedness is a key feature of the global financial system. Understanding how financial shocks experienced by certain companies or sectors can spread, potentially leading to wider crises, is self-evidently of interest to policy-makers, investors and business owners. We employ methods from network science, together with epidemic modelling and Extreme Value Theory, to create and analyse financial shock propagation models.

We use stock price data for a set of 239 companies to construct a multilayer dynamic network using tail dependence coefficients to measure the risk that two companies suffer together and propose a framework for modelling financial contagion using an SIR (susceptible-infected-recovered) epidemic model. The method is based on a stochastic epidemic transmission mechanism, in which shock can be propagated both locally (to neighbours in the network) and globally (to any company). We identify which companies have suffered during a particular time period using stock price volatility. Our focus is then on simulating how the shock spreads from the initially infected companies to the rest by considering their connectivity at the local and global level. We fit the model to the 2 most recent crises, the 2008 financial crisis and 2020 crisis, and we explore and quantify its utility to predict spread of financial shock through the network. The model successfully reproduces the number of affected companies in each crisis. Keywords: network science, financial contagion spread, epidemic modelling, statistical analysis

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From Mice, to Machine, to Man: The mathematics and computing of clearance in Alzheimer's disease

Georgia S. Brennan

University of Oxford

A. Goriely (University of Oxford), M. E. Rognes (Simula Research Laboratory), T. B. Thompson (University of Oxford)

Every three seconds, at least one person is diagnosed with dementia; the most common form of dementia is Alzheimer's disease (AD) and the most significant risk factor for AD is age. In first world countries, 18-30% of people are 60+ and AD is now a leading cause of death and economic burden across the globe. To beat AD, we must understand our options for intervention. Contemporary medical research suggests that the brain's ability to clear waste proteins plays a central role in AD pathogenesis and progression. Though the data in animal models are promising,

testing any of these observations in humans is challenging. My research delivers data-driven mechanistic mathematical models and powerful scientific computing tools that bring together the mechanism of clearance with the prion-like dynamics of the misfolded proteins characterising AD progression. A key finding of my work is that that the coupling between proteopathic spreading and regional brain clearance may not only alter the trajectory of AD, but also provide a potential window into AD subtypes. Mathematics can bridge the gap from mice to machine to man in AD research. Keywords: Mathematical Modelling, Mathematical Biology, Dynamical Systems, Alzheimer's disease

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The Linear Stability of Ferrofluids Subject to Non-Uniform Magnetic Fields

Sarah Ferguson Briggs
Imperial College London
Jonathan Mestel

The linear stability of Newtonian ferrofluids subject to non-uniform magnetic fields is investigated in different configurations. Both linear and field-dependent susceptibilities are considered. Of particular interest are configurations with non-constant susceptibility, when for an equilibrium the field is a function of the susceptibility. It is argued that such equilibria are unstable if ever the gradient of the field and the gradient of the susceptibility point in different directions, but stable if the gradients are everywhere aligned. Keywords: Ferrofluids, Ferro-hydrodynamics, Linear Stability Analysis

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Dynamic tipping in the non-smooth Stommel-box model for thermohaline circulation

Chris Budd
University of Bath
Rachel Kuske, Georgia Tech

In this talk I will describe the behaviour at tipping points close to non-smooth fold bifurcations in non-autonomous systems. The focus will be the Stommel-Box, and related climate models, which are piecewise-smooth continuous dynamical systems, modelling thermohaline circulation. I will obtain explicit asymptotic expressions for the behaviour at tipping points in the settings of both slowly varying freshwater forcing and rapidly oscillatory fluctuations. The results, based on combined multiple scale and local analyses, provide conditions for the sudden transitions between temperature-dominated and salinity-dominated states. In the context of high frequency oscillations, a multiple scale averaging approach can be used instead of the usual geometric approach normally required for piecewise-smooth continuous systems. The explicit parametric dependencies of advances and lags in the tipping show a competition between dynamic features of the model. We make a contrast

between the behaviour of tipping points close to both smooth Saddle Node Bifurcations and to non-smooth systems. In particular we show that the non-smooth case has earlier and more abrupt transitions. This result has clear implications for the design of early warning signals for tipping in the case of the non-smooth dynamical systems which often arise in climate models. Keywords: Climate change, Tipping Points, Non-smooth dynamical systems

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Deformation of swelling and shrinking bilayer beams

Matthew Butler

University of Birmingham

Tom Montenegro-Johnson (University of Birmingham)

Responsive hydrogels are a promising material for creating controllable actuators for use on micro-scale devices, because they expand and contract significantly in response to external stimuli. This size change can be exploited to generate controllable structural shape changes in inhomogeneous materials, since differential swelling generates internal stresses that are relaxed by deformation. We consider one of the most basic inhomogeneous structures, the bilayer beam, but allow the material properties to vary along its length. A simple mathematical model reveals the resulting beam curvature as the material swells, which we compare to known classical results for bilayer beams.

Keywords: Swelling, beams, hydrogels

Emergent probability fluxes in confined microbial navigation

Jan Cammann

Loughborough University

Fabian Jan Schwarzendahl (Heinrich-Heine-Universität Düsseldorf), Tanya Ostapenko (Max Planck Institute for Dynamics and Self-Organization), Danylo Lavrentovich (Max Planck Institute for Dynamics and Self-Organization), Oliver Bäumchen (University of Bayreuth), Marco G. Mazza (Loughborough University)

In recent years, biological microswimmers have attracted considerable interest due to the biological and ecological implications of understanding the mechanisms governing their dynamics. The possibility to harness their motion to power microdevices is a topic of exceptional importance for modern microtechnology. When the motion of a motile cell is observed closely, it appears erratic, and yet the combination of nonequilibrium forces and surfaces can produce striking examples of organization in microbial systems. Most of our current understanding is based on bulk systems or idealized geometries, it remains elusive how and at which length scale self-organization emerges in complex geometries. We use experiments, analytical and numerical calculations to study the motion of motile cells under controlled microfluidic conditions, and demonstrate that probability flux loops organize active

motion even at the level of a single cell exploring an isolated compartment of non-trivial geometry. By accounting for the interplay of activity and interfacial forces, we find that the boundary's curvature determines the nonequilibrium probability fluxes of the motion. We theoretically predict a universal relation between fluxes and global geometric properties that is directly confirmed by experiments. Our results represent a general description of the structure of nonequilibrium fluxes down at the single cell level opening the possibility to decipher the most probable trajectories of motile cells and may enable the design of geometries guiding the time averaged motion of microswimmers. Keywords: microswimmers; chlamydomonas; nonequilibrium; motility; algae

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Modelling spatial and phenotypic heterogeneity in solid tumours in the presence of radiation therapy

Giulia Laura Celora

University of Oxford

Prof Helen Byrne (University of Oxford); Prof Panayotis Kevrekidis (University of Massachusetts Amherst)

In cancer, treatment failure and disease recurrence have been associated with the heterogeneous composition of tumours, where cells with different phenotypic properties (such as sensitivity to treatment) coexist. In this talk I will present a structured-population model to describe the evolution of tumour heterogeneity in a slice of tissue which is oxygenated from the boundary by a vessel and exposed to radiation treatment. The model consists of a system of coupled non-local partial differential equations that links the phenotypic evolution of tumour cells to the local oxygen levels and treatment. I will start by showing how numerical bifurcation analysis can be applied to study the long-time behaviour of the system in the absence of treatment. For biologically relevant parameter values, the system exhibits multiple steady states in the absence of treatment; in particular, depending on the initial conditions, the tumour is either eliminated ("tumour-extinction") or it persists ("tumour-invasion"). Using dynamic simulations, I will then discuss how radiotherapy can be applied to drive an invading tumour (where radio-resistant cells are originally present) to extinction. The results presented give insight on how phenotypic heterogeneity evolves during treatment and highlight the link between the oxygen distribution in the tissue and the efficacy of different radiation schedules commonly used in clinical settings.
Keywords: mathematical biology; phenotypic-structured models; cancer

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Existence and Smoothness of the Navier-Stokes equation by a Boundary Integral representation

Dr. Edmund Chadwick
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Consider a published solution by the author for the Navier-Stokes equation by a boundary integral velocity representation of fundamental solutions called NSlets in a four-dimensional space-time domain. Here, we show that the strength of the fundamental solutions is the force impulse distribution, and the near-field asymptotic of the NSlet is the Eulerlet. So equivalently, the velocity is asymptotically close to a near-field boundary integral distribution of Eulerlets. Considering this representation, it is shown that if the force impulse generating the motion is bounded, then the velocity is bounded and exists. Conversely, if the force impulse is unbounded, then a solution does not exist. Furthermore, making use of the smoothness property of the Eulerlets, it is shown that this solution is also smooth. It is noted that the Eulerlet is unstable as it assumes flow slips without friction. Physically, this instability gives rise to turbulent flow. Furthermore, the Eulerlet is time-reversible. This means in the local approximation a time stepping model could generate a finite time singularity, which is not the case for the boundary integral model presented here.

Keywords: Navier-Stokes equation, boundary integral method, fundamental solutions

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Spontaneous pattern formation with Salerno equations: ring-cavity feedback, static instabilities, and mean-field theory

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In physics, the discrete nonlinear Schrödinger (dNLS) equation plays a key role in modelling wave propagation in periodic optical systems [Christodoulides and Joseph, Opt. Lett., vol. 13(9), 794-796 (1988)]. Architectures typically involve light confined to a set of waveguide channels with nearest-neighbour coupling and whose dielectric response has a local cubic nonlinearity. While the widely-used dNLS model is non-integrable, it possesses an integrable counterpart–the Ablowitz-Ladik (AL) equation [J. Math. Phys. vol. 17(6), 1011-1018 (1976)]–which is often of greater interest in applied mathematics research. The price paid for integrability is a nonlinear response that remains cubic but becomes nonlocal in a way that defies straightforward physical interpretations. In this presentation, our interest lies with the Salerno equation [Phys. Rev. A, vol. 46(11), 6856-6859 (1992)], which facilitates a simple linear interpolation between the dNLS and AL regimes.

Here, we consider the Salerno equation in the context of spontaneous pattern formation involving a discrete waveguide array and a ring-cavity arrangement. Feedback from the cavity–which comprises external periodic pumping, coupling-mirror losses, and mistuning relative to the pump wave–is accommodated via a single 'lumped' boundary condition applied on the input plane. The stationary plane-wave solutions of the cavity are detailed, and a linearized perturbation theory deployed to predict their robustness against small-amplitude periodic modulations. In this way, the most-unstable spatial frequency (hence the dominant length-scale of any emergent static patterns) can be identified from the threshold instability spectrum. The dNLS and AL spectra appear as special cases, and the long-wavelength asymptotics of all three models are consistent with the continuum nonlinear Schrödinger equation.

Extensive simulations of discrete cavities with a single transverse dimension have been carried out, with initialization corresponding to a plane-wave stationary state perturbed by low-level coloured noise. Those numerical calculations demonstrate the emergence of static cosine-type patterns, in good agreement with theory. We have also extended our considerations to capture a second transverse dimension in the Salerno equation. Simulations have yielded static hexagon patterns that appear to be stable across time.

We conclude with a foray into mean-field theory, which is typically used to model the space-time dynamics of a longitudinally-averaged cavity field. The resulting Salerno equation is of the discrete Ginzburg-Landau class, where cavity effects appear as additional forcing terms rather than through repeated application of a formal boundary condition. Results from pattern formation in both one and two transverse dimensions will be detailed. Keywords: Discrete equations, instabilities, nonlinear waves, pattern formation.

Young and Young-Laplace equations for a static ridge of nematic liquid crystal, and transitions between equilibrium states

Joseph R. L. Cousins

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Joseph R. L. Cousins, Brian R. Duffy, Stephen K. Wilson and Nigel J. Mottram

Situations involving interfaces between a nematic liquid crystal (nematic), a solid substrate, and a passive gas that includes nematic-substrate-gas three-phase contact lines are of great interest, both scientifically and technologically. In particular, in recent years, the push to exploit the interfacial, dielectric, and viscoelastic anisotropies of nematics has led to the development of devices used in flow processing, microelectronic production, and adaptive-lens technologies that extend beyond the well-known application of nematics in liquid crystal displays. Understanding many of these emerging technologies, which often involve nematic droplets or films, requires a theoretical description of the wetting and dewetting phenomena of nematics. To further understand wetting and dewetting phenomena for nematics, we analyse a two-dimensional static ridge of nematic liquid crystal (nematic) resting on a solid substrate in an atmosphere of passive gas [1]. Specifically, we obtain the first complete theoretical description for this system, including nematic Young and

Young-Laplace equations. Then, under the assumption that anchoring breaking occurs in regions adjacent to the contact lines, we use the nematic Young equations to determine the continuous and discontinuous transitions that occur between the equilibrium states of the ridge. In particular, in addition to continuous transitions analogous to those that occur in the classical case of an isotropic liquid, we find a variety of discontinuous transitions, as well as contact-angle hysteresis, and regions of parameter space in which there exist multiple equilibrium states for the ridge that do not occur in the classical case [1]. The range of anisotropic wetting and dewetting phenomena found in this nematic system may also be useful for understanding many emerging technologies using nematic materials.

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[1] Joseph R. L. Cousins, Brian R. Duffy, Stephen K. Wilson, Nigel J. Mottram. Young and Young-Laplace equations for a static ridge of nematic liquid crystal, and transitions between equilibrium states. arXiv:2111.07741, 2021

Keywords: nematic liquid crystals; wetting; dewetting; Young equation; Young-Laplace equation

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The use of exponential asymptotics versus Borel summation in studying singularly perturbed differential equations

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Philippe Trinh

Since the end of the twentieth century, it has been shown that a number problems require the derivation of beyond-all-orders terms (often exponentially small) for the resolution of some physical effect. These problems include those related to the study of dendritic crystal growth, Saffman-Taylor viscous fingering, water waves, localised pattern formation, and solitons in quantum theory. Primarily in the UK and amongst applied mathematicians and physicists, this has motivated the development of exponential asymptotics. More globally, however, there are many other areas in pure and applied mathematics that relate to the study of asymptotic divergence. These include: hyperasymptotics, resurgence, exact WKB analysis, and Borel summation. The differences and similarities between these different areas and styles of analysis are often obscure or incomplete.

In this talk, we elucidate the relationship between exponential asymptotics and Borel summation, as applied to the analysis of singularly perturbed ODEs. We introduce the analogue of the late terms ansatz by positing certain singularities in the Borel plane and use the framework to construct a number of new problems in applied exponential asymptotics that are, in some sense, exactly soluble. Our work also allows rigorous demonstration of certain aspects of the exponential asymptotics procedure – such as a derivation of Van Dyke's matching rule. Keywords: asymptotic analysis

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A Model for Ultrasonic Transducers with Boundary Dynamics in a High-Temperature Regime

Michael Doherty

University of Strathclyde

Marcus Waurick, Technische Universitt Bergakademie Freiberg

Ultrasonic transducers are devices which are both ubiquitous in application and the subject of much contemporary interest. Applications range from non-destructive testing to medical imaging and beyond. Yet, the mathematical modelling of these devices often focuses on their piezo-electromagnetic properties and neglects the effects of a high-temperature regime. In this talk I will present an abstract model to describe ultrasonic transducers taking into account the effects of high-temperature and a range of boundary conditions. Here, the system describing ultrasonic transducers (a set of coupled thermo-piezo-electromagnetic equations) is extended with tools from abstract boundary data spaces in order to encode boundary conditions within the system. The aim of the model is to highlight those systems which are well-posed as evolutionary equations (i.e. both Hadamard well-posed and causally dependent on the data). After showing how the model accommodates both Robin and non-standard inhomogeneous boundary conditions (like those of impedance- or Leontovich-type), I will address the question of evolutionary well-posedness for the system when taken together with a particularly interesting set of boundary conditions. Keywords: coupled systems; well-posedness; Maxwell's equations; dynamic boundary conditions; PDEs

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Pore-network models for haematocrit transport in disordered porous domains reflecting the human placenta

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Qi Zhou[2], Miguel O. Bernabeu[3], Timm Krüger[2], Oliver E. Jensen[1], Igor L. Chernyavsky[1,4], 1 Department of Mathematics, University of Manchester, 2 School of Engineering, Institute for Multiscale Thermofluids, University of Edinburgh, 3 Centre for Medical Informatics, Usher Institute, University of Edinburgh, 4 Maternal and Fetal Health Research Centre (School of Medical Sciences), University of Manchester

The placenta enables the transport of oxygen and nutrients to the fetus from the mother. The human placental circulatory system consists of separate maternal and foetal blood flows over a complex 3D domain of porous regions and capillaries. The oxygen transport mechanisms in the maternal placenta are fundamentally linked with the flow of red blood cells (RBCs) and the highly heterogeneous topology of the maternal domain within the placenta. Here we use a continuum description of the suspension flow of RBCs through disordered porous media to understand the impact of geometry on RBC transport.

Disordered 2D domains are constructed by randomly placing non-overlapping circles on a region until saturation is reached. Voronoi tessellation and Delaunay triangulation are then used to construct a series of pores and throats throughout the domain. Using a pore-network model, flux is evaluated along each throat and haematocrit, the volume fraction of RBCs present in the flow, is evaluated at each pore. Experimental observations have long demonstrated the variable viscosity of blood and unequal splitting of haematocrit at bifurcations within networks where the size of the vessel approaches that of the diameter of a RBC, (T.W. Secomb, Annu Rev Fluid Mech, 49:443-46, 2017). These physical observations are incorporated into the modelling framework by using empirical relationships based on variation from Newtonian plasma flow. Results are compared against high performance computing simulations utilising lattice Boltzmann and immersed boundary methods.

The continuum empirical setup for suspension flow of RBC in this works allows for a discussion on the impact of the presence of RBCs on overall porous flow properties. The effects and physical interpretation of variables in this setup are investigated. This work extends the pore-network model approach to incorporate complex non-Newtonian flow descriptions and has the potential to uncover the structure-dependent mechanisms within blood flow in porous biological tissues such as the placenta.

Keywords: haemodynamics, biological tissue, porous media, non-Newtonian flow, pore-network modelling

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Using an agent-based model to simulate recurrent urinary tract infections

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Ruth Bowness (University of Bath), Tommaso Lorenzi (Politecnico di Torino), Ben Parcell (NHS Tayside)

Urinary Tract Infections (UTIs) are amongst the most common infections worldwide, affecting well over 150 million people each year. UTIs now account for 40% of all hospital-acquired infections and they are becoming harder to treat, with an estimated 1 in 3 being resistant to the most commonly used antibiotics. UTIs are also notorious for recurring. Using agent-based modelling techniques we have developed a model that describes the infection process in recurrent urinary tract infections (rUTIs). Gaining a better understanding of the pathophysiology can prove key to the development of new treatment strategies with greater success and less resistance rates. Data arising from animal and cell culture models are incredibly valuable but can be limited by ethical considerations and time constraints. Simulations from in silico models can be analysed and their results can complement clinical findings, adding to the understanding of how the infection behaves and how we might improve treatment. We initially model a lower urinary tract infection, focusing on a section of the bladder. We simulate discrete agents in the system: Escherichia coli bacteria and the immune cell types reported to have critical roles in lower UTIs (LY6C macrophages and mast cells). The capacity of the bacteria to penetrate the bladder epithelial barrier and seek refuge in the bladder epithelial cells is a critical initiating step of infection and this process is simulated in our model. Keywords: mathematical biology

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A mathematical model reveals complex roles of platelets in hepatitis progression and resolution

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Hepatitis is the term used to describe inflammation in the liver. It is associated with a high rate of mortality, but the underlying disease mechanisms are incompletely understood and treatment options are limited. We developed a new mathematical model of hepatitis to understand the complex interactions between hepatocytes (liver cell), hepatic stellate cells (cells in the liver that produce hepatitis-associated fibrosis) and immune cells that mediate inflammation. Recent work has highlighted a role for platelets, blood cells that are recognised to trigger blood clotting following injury, in the resolution of liver inflammation and we extend the model to incorporate such effects.

The model is in the form of a system of ordinary differential equations. We use numerical techniques and bifurcation theory to characterise and elucidate the physiological mechanisms that dominate liver injury and its outcome to a healthy or unhealthy, chronic state. Simulations and bifurcation analysis revealed the opposing roles that platelets play, demonstrating an early pro-inflammatory effect, but at later time points an anti-inflammatory role in which they support disease resolution.

This study reveals the complex interactions between multiple cell types involved in this complex disease and highlights potential problems in targeting platelets to treat established disease.

Keywords: Bistable, bifurcations, biology

Direct and inverse Solutions for non-homogeneous Wave Equations with Unusual Boundary Conditions

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In science and technology, the inverse wave problem, which in this study's focus, can appear in the vibration of materials, implosion, explosion, and earthquake, etc. In physics, geophysics, and engineering, dealing with wave, wind, seismic, explosion, or

noise excitations, also leads to this type of problem. In recent years, research on inverse problems has become more popular especially those involving the identification of heat/force source coefficients, as we can see in recent work done by Huntul and Tamsir (2020). Tekin (2019 and 2020) has reconstructed a time-dependent potential function in a wave equation subject to unusual boundary conditions, and he has also studied the existence and uniqueness of the potential solutions. Siskova and Slodicka (2018) have studied the inverse source problem solutions when non-traditional dynamical boundary conditions are considered. Hussein (2021) has recently published a paper that studies the inverse solutions of wave problems which consider the upper-based initial condition as over-determination data.

This research examines the inverse source wave problem in two chosen cases, the first investigating the impact of involving a new type of unusual boundary condition on the accuracy, stability, and convergence of the direct and inverse solutions. The other case concerns the potential impact of moving Dirichlet data to the right with a left/right Neumann condition as extra data. The research is a significant development and it supplements the work of Hussein (2020) which studied non-local boundary conditions plus the displacement boundary condition as the additional measurements. This work involves testing and re-assessing various coefficients involved within the equation and its conditions in the unusual boundary case and seeing how far this works compared to those in Hussein, and Lesnic (2014, 2016) & Tekin (2019). To clarify such evolutions, numerical examples have been examined. We will integrate the separation of variables method with the finite difference method to and direct solutions for problems in both proposed cases. Then, the solutions obtained from solving the direct problem are used to reconstruct the force source parameters which is a space-dependent function. To stabilise the inverse solutions, the zeroth, first, and second-order Tikhonov regularization methods will be considered. This will achieve better-approximated solutions, especially in the case where the left-end flux tension is measured. We will include and discuss useful numerical examples and explore some theories that ensure the existence, uniqueness, and stability of the solution.

The detailed references list is available upon your request. Keywords: Numerical analysis, Inverse problems, Finite difference methods, and Tikhonov regularization methods

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Three linked spheres microrobotic steady and oscillating motions at low Reynolds number

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Microrobots have grown in importance with a variety of applications in various fields, some of the most important and significant of which can be found in the field of medicine [1]. Najafi and Golestanian [2] introduced a simple swimmer based on a small number of linked spheres model swimmers and demonstrated that it works well at low Reynolds number. In this talk we will present firstly, results of steady solution and a translational vibration solution by considering translational small-amplitude vibration of a sphere moving in a uniform flow field at low Reynolds number. The steady solution is given by the near-field Stokes flow past a sphere with a matching far-field Oseen flow. The translational vibration solution is a near-field Stockes flow given by Pozrikidis [3] in terms of an unsteady Stokeslet and quadrupole. we give the matching far-field Oseen flow by an unsteady Oseenlet and quadrupole. The solution is visualized by using MATLAB and shown to agree with existing solutions when the frequency of vibration tends to zero (steady solution), and when the far-field length tends to zero (Pozrikidis near-field solution). Secondly, from these results, we will present a solution for three linked spheres by calculating the hydrodynamic interaction Oseen tensor between spheres for steady and oscillating motions following the approach of Najafi [2] and Hossein [4].

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Keywords: Keywords: Microrobot; Three spheres; steady and translational flow past a sphere, Low Reynolds number; small amplitude vibration of sphere; uniform flow field; far-field Oseen quadrupole; hydrodynamic interaction Oseen tensor.

A systematic upscaling of mass transport models for organoid expansion via homogenisation

Meredith Ellis

University of Oxford

Prof Sarah Waters (University of Oxford), Prof Helen Byrne (University of Oxford), Dr Mohit Dalwadi (UCL), Prof Marianne Ellis (University of Bath, Cellesce Ltd), Mr William Newell (Cellesce Ltd)

Organoids are three-dimensional multicellular tissue constructs used in applications such as drug testing and personalised medicine. We are working with the biotechnology company Cellesce, who develop bioprocessing systems for the expansion of organoids at scale. They have developed a bioreactor, in which organoids are embedded within a layer of hydrogel and a flow of culture media across the hydrogel is utilised to enhance nutrient delivery to, and facilitate waste removal from, the organoids. A complete understanding of the system requires spatial and temporal information regarding the relationship between flow and the resulting metabolite concentrations throughout the bioreactor. However, it is impractical to obtain these data empirically, as the highly-controlled environment of the bioreactor poses difficulties for online real-time monitoring of the system. Mathematical modelling can be used to improve the yield of organoids grown within the bioreactor, by predicting the metabolite concentrations during culture for different operating conditions.

However, since millions of discrete organoids are grown simultaneously, modelling the mass transport and organoid growth is computationally challenging for this multiply connected, three-dimensional problem which involves tracking many moving boundaries located at the interface between the organoids and the hydrogel.

We present a general mathematical model for the transport of nutrient to, and removal of waste metabolite from, organoids growing within the hydrogel. We use an asymptotic (multiscale) approach to systematically determine effective equations that govern the macroscale mass transport. We use the homogenised equations to explore different culture conditions within the bioreactor and show how they influence mass transport within the hydrogel. In this way, we highlight the important role played by flow in enhancing metabolite transport and, consequently, improving organoid growth. Keywords: organoid culture; multiscale; mathematical model; homogenization; mass transport; bioreactor

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Pharmacokinetic Modelling for Adrenal Support

Rosie Evans

University of Birmingham

Professor David Smith, University of Birmingham

Current cortisol dosing regimes for patients with adrenal insufficiency are unable to accurately replicate the physiological profile of healthy patients. Endocrinological mathematical models aim to bridge this gap by allowing for the prediction of different treatment strategies to circumvent clinical trials. We present a simplified model of hydrocortisone delivery via oral tablets, intravenous bolus, and continuous intravenous infusion. The model is formulated in terms of linear kinetics and considers the dynamics of glucocorticoid-protein binding. To validate our model, we also test whether it can replicate a healthy patient response. The models are fitted to recently published data on 50 mg dosing every 6 hours (or a 200mg continuous infusion) and healthy patient data. We then introduce a different model to fit the biological response more accurately in the continuous infusion case; specifically, we consider production and degradation of a cortisol-removal enzyme to better match the long time-scale equilibrium seen in patient data. Finally, our model parameters are estimated using Bayesian inference with the software Stan. Keywords: Pharmacokinetic Modelling, ODEs, Bayesian Inference

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Combining Dynamic Mode Decomposition with Ensemble Kalman filtering for tracking and forecasting

Stephen Falconer

University of Surrey

David Lloyd, Naratip Santitissadeekorn

Data assimilation techniques, such as Ensemble Kalman Filtering, have been proven to be a highly effective and efficient way to combine noisy data with a mechanistic model to track and forecast systems. However, when dealing with high-dimensional data it is often difficult to derive a mechanistic model, making data assimilation difficult to apply. In this talk, we use Dynamic Mode Decomposition to generate a low-dimensional, linear model of a dynamical system directly from high-dimensional data which is defined by temporal and spatial modes. We then combine Dynamic Mode Decomposition with the Ensemble Kalman Filter (which we call the DMDEnKF) to iteratively update the current state and temporal modes as new data becomes available. We demonstrate that this approach has the advantage of being able to track time varying dynamical systems in synthetic examples. We then apply the DMDEnKF to influenza-like illness data from the USA Centers for Disease Control and Prevention. Keywords: Dynamical Systems, Data driven methods, Data Assimilation, Dynamic Mode Decomposition, Ensemble Kalman Filter

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Modelling Differentiating Stem Cells: A Novel View

Saeed Farjami

University of Surrey

Karen Camargo Sosa (University of Bath), Jonathan H.P. Dawes (University of Bath), Robert N. Kelsh (University of Bath) and Andrea Rocco (University of Surrey)

Understanding the underlying mechanism(s) in cell fate selection is a big challenge in developmental biology. For a long time, the main view on differentiating stem cells has been based on the epigenetic landscape metaphor proposed by Waddington in 1957. However, in recent years, the experimental data, obtained using more advanced methods, questions this idea. In contrast, recent views support a more dynamic process during embryonic development preserving the multipotency until the late stages of cell specification. Here, we propose a class of simple mathematical models with oscillatory behaviours using ordinary differential equations (ODEs). We present a bifurcation analysis of the model and explain the entering and exiting mechanisms into and out of the oscillatory regime under two different scenarios. First, only one single signalling pathway (control parameter) drives the system; second, multiple signalling pathways (parameters) are involved in pushing the system into and out of the oscillations. Finally, we consider the stochastic version of the ODE model to study the effect of intrinsic noise. Keywords: stem cell, multipotency, gene expression, gene regulatory network, differentiation, oscillation

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Modelling Encapsulated Stem Cells For Non-Invasive Therapy In The Liver

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In 2020, cirrhosis and other liver diseases were among the top five causes of death for individuals aged 35-65 in Scotland, England and Wales. At present, the only curative treatment for end-stage liver disease is through transplant which is unsustainable. Stem cell therapies could provide an alternative. By encapsulating the stem cells we can modulate the shear stress imposed on each cell to promote integrin expression and improve the probability of engraftment. We model an individual, hydrogel-coated stem cell moving along a fluid-filled channel due to a Stokes flow. The stem cell is treated as a Newtonian fluid and the coating is treated as a poroelastic material with finite thickness. In the limit of a stiff coating, a semi-analytical approach is developed which exploits a decoupling of the fluids and solid problems. This enables the tractions and pore pressures within the coating to be obtained, which then feed directly into a purely solid mechanics problem for the coating deformation. We conduct a parametric study to elucidate how the properties of the coating can be tuned to alter the stress experienced by the cell. Keywords: Asymptotics; Poroelasticity; Hydrogels; Biological flows.

Fluctuation-driven transitions in finite time: beyond asymptotic rates for rare events

Steve Fitzgerald

University of Leeds

AJ Archer, Loughborough University; AB Hass, University of Leeds

Fluctuation-driven rare events, such as chemical reactions traversing an activation barrier, or crystal defects migrating through a material, have low probability of occurrence yet dominate the outcome of many physical, chemical, and biological processes. Their direct simulation (e.g. using molecular dynamics) is notoriously difficult because they so rarely occur on computationally-accessible timescales. Many techniques have been developed to study these events, and most focus on determining the average rate at which they occur (typically by calculating an asymptotic average in the long-time limit). One important approach is to determine the path through the potential energy surface from initial to final state with the minimum hill-climbing required, then apply Kramers'-type rate theory to the process of crossing these barriers. However, this only corresponds to the most probable path in the long-time limit, and whether or not the timescales of interest are long enough depends on the process. We show that enforcing the constraint of finite time can lead to a rich phenomenology of radically different transition pathways, that cross

different barriers, corresponding to different intermediate states. In this talk we will introduce the path- (functional) integral formulation of stochastic processes [1] we use to enforce the time constraint, and present a generalization of the geometric minimum action method [2] to find the most probable path.

[1] Graham, R., 1977. Path integral formulation of general diffusion processes. Zeitschrift fr Physik B Condensed Matter, 26(3), pp.281-290. [2] Vanden-Eijnden, E. and Heymann, M., 2008. The geometric minimum action method for computing minimum energy paths. The Journal of chemical physics, 128(6), p.061103.

Keywords: stochastic processes; rare events; path integrals

Mathematical modelling of metal rolling: the role of elastic and plastic deformation

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Metal production generally involves four stages: ore extraction, smelting, casting and forming. We focus here on the final stage, metal forming, and in particular on the process known as metal rolling. The goal of this process is to reduce the thickness of a sheet of metal. To achieve this, the sheet is passed between two rotating rollers which are held in fixed positions and which indent the sheet. A key ingredient for successful implementation of metal rolling is understanding the roles of plastic (permanent) deformation and elastic (reversible) deformation: as the sheet loses contact with the rollers, elastic springback leads to an increase in thickness compared to the thickness imposed by the rollers.

In this talk we will present a mathematical model for metal sheet rolling, taking both elastic and plastic behaviours into account. We consider a thin-sheet limit, which yields one-dimensional purely plastic behaviour at leading order. Careful consideration of correction terms and a comprehensive boundary layer analysis are required to resolve cross-thickness variation and elastic springback. This is complicated by the need to determine both where the sheet is in contact with the rollers and where the sheet deforms elastically versus plastically. Numerical simulations carried out in Abaqus will provide further insight. Keywords: Asymptotic analysis, elastic and plastic deformation, metal forming

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Feedback control of propagating bubbles in Hele-Shaw channels

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Alice B. Thompson - Department of Mathematics, The University of Manchester

We explore the capabilities of feedback control to stabilise and manipulate propagating bubbles in the confined geometry of a rectangular Hele-Shaw channel. Several steadily-propagating solution branches exist in this system, with only one linearly stable and subsequent branches featuring increasingly deformed bubble shapes and increasing numbers of unstable eigenmodes. Our aim is to use feedback control and control-based continuation to detect and stabilise at least the first of these unstable branches. This system is an appealing prototype for control: the low Reynolds number and strongly confined geometry means the system state is essentially encapsulated in the interface shape as viewed from above, recent experimental realisations of this system are in good agreement with depth-averaged models, and the system responds well to actuation via fluid injection, but nonetheless practical implementation of feedback control presents significant challenges. In this talk, we use a depth-averaged model to illustrate how control would work in this system, including the design of a suitable gain matrix, the impact of control on the bifurcation structure, the complexities of controlling a propagating bubble moving past a fixed array of injection points, and how this idealised simulation relates to experimental reality. Keywords: Hele-Shaw flows, Control based continuation, Flow control

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Dynamical effects of electromagnetic flux on Chialvo neuron map: nodal and network behaviors

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This is a study of the dynamical effects of the application of electromagnetic flux on discrete Chialvo neuron (https://arxiv.org/abs/2201.03219). I will talk about how the model manifests rich dynamical behaviors like multistability, firing patterns, antimonotonicity, closed invariant curves, various routes to chaos, and fingered chaotic attractors. I will next talk about how we have adopted the traditional techniques of bifurcation diagrams, Lyapunov exponent diagram, phase portraits, basins of attraction, and numerical continuation of bifurcations to confirm the dynamical behaviors exhibited by the system. Finally, I will shift my discussion from a single neuron to a network of Chialvo neurons and will end the talk by exploring how different dynamical regimes such as synchronous, asynchronous, and chimera states are revealed. Keywords: discrete dynamical system; neuron systems; routes to chaos; networks; chimera state

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Modelling the MIEX water treatment process

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University of Strathclyde

Jozsef Farkas (University of Stirling), Geraldine Knops (United Utilities Group PLC), Nigel Mottram (University of Glasgow)

We present a hierarchy of models for the operation of the magnetic ion-exchange resin water treatment process. We use the modelling framework introduced in arXiv:2102.06490. The starting point is a transport equation governing the evolution of resin particles coupled to an integro-differential equation for the dissolved organic matter. We discuss the modelling framework, existence of solutions and uniqueness of equilibrium states. Keywords: waste water treatment, transport equations, structured population models

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Reduction of Leading-Edge Noise by Tailored Turbulence Anisotropy

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This paper investigates the effect of anisotropic turbulence on the generation of leading-edge aerofoil-turbulence interaction noise, and further considers the dual impact of anisotropy in conjunction with an acoustically compliant (porous) edge. Thin aerofoil theory is used to model an aerofoil as a semi-infinite plate and the scattering of incoming turbulence is solved via application of the Wiener-Hopf technique. In the case of a compliant plate modelled as having an impedance boundary condition, a useful numerical formulation for the Maliuzhuinets function forms an important component of the solution. This theoretical solution encapsulates the diffraction problem for gust-aerofoil interaction, and is integrated a wavenumber-frequency spectrum to account for general incoming turbulence. The specific wavenumber-frequency spectrum in the anisotropic case is obtained using the method of Gaussian decomposition, in which the generalized spectra is approximated through the weighted sum of individual Gaussian eddy models. We compare our results against experimental measurements and see good agreement. Keywords: Leading Edge Noise, Noise Control, Aeroacoustics, Turbulence Spectra

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Efficient detection of twinning in crystallographic data using modified Rodrigues parameters

Cameron Hall

University of Bristol

Laura Midgley (Durham), Christian Boehmer (UCL), Norbert Peyerimhoff (Durham), and Horst Puschmann (OlexSys)

Diffraction methods such as X-ray crystallography are powerful tools for determining the atomic structure of crystalline materials. However, certain crystal defects such as twinning can make diffraction data much harder to interpret. In the absence of twinning, a diffraction experiment produces a three-dimensional lattice of intensities that encode information about the unit cell of the crystal. When twinning occurs, the experimental data will contain both the true data (as for the untwinned crystal) and a rotated version of the true data. If this rotation causes data points associated with twinning to be overlaid on data points from the true crystal, the twinning needs to be identified and removed from the data before they are used for structural elucidation. Given only the experimental diffraction data from a twinned crystal, it is computationally challenging to identify the 3D rotations from twinning that could lead to these problems.

In this talk, I will present a new method for identifying the 3D rotations that could give rise to diffraction data points being overlaid on each other. This method depends on the representation of 3D rotations using "Modified Rodrigues Parameters" (MRPs), which are stereographic projections of the unit quaternions into 3D Euclidean space. Using MRPs, we have developed a computationally efficient method that determines which rotations of a 3D lattice could lead to some or all of the rotated datapoints being within a given tolerance of the original datapoints. I will discuss how the method works and illustrate the method by applying it to real data from a twinned crystal. Keywords: materials science; quaternions; 3D rotations; computational methods; iterative bounding

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The Formation of Wildfire Fingers

Sam Harris

University College London (UCL)

Robb McDonald - UCL

Wildfires are among the deadliest natural disasters the planet faces, and as the effects of climate change worsen, they are becoming increasingly more common across the globe. In the UK, recent, notable examples include: the 2018 Saddleworth Moor Fire (England) and the 2019 Moray wildfire (Scotland). Predicting how wildfires will spread is vital in protecting homes, preserving wildlife and saving lives. In this talk, three key mechanisms of wildfire spread - constant rate of spread, curvature and oxygen effects - are introduced and a resulting two-dimensional model is constructed. The oxygen effect, which is not seen explicitly in previous wildfire models, is dynamical and requires the solution of the steady advection-diffusion equation.

This adds a destabilising effect to the fire line - the free boundary separating burnt and unburnt regions - causing the development of so-called “fire fingers”, analogous to the problem of viscous fingering in a Hele-Shaw cell. To finish, numerical solutions are computed using a conformal mapping method. Keywords: free surface (interfacial) flows, fingering instability, wildfire spread

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Bayesian inference on a microstructural, hyperelastic model of tendon deformation

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Dr Simon Cotter; Department of Mathematics, University of Manchester. Professor William J. Parnell; Department of Mathematics, University of Manchester. Dr Tom Shearer; Department of Mathematics & Department of Materials, University of Manchester.

Microstructural models of soft tissue deformation are important in applications including artificial tissue design and surgical planning. The basis of these models, and their advantage over their phenomenological counterparts, is that they incorporate parameters that are directly linked to the tissue’s microscale structure and constitutive behaviour and can therefore be used to predict the effects of structural changes to the tissue. Although studies have attempted to determine such parameters using diverse, state-of-the-art, experimental techniques, values ranging over several orders of magnitude have been reported, leading to uncertainty in the true parameter values and creating a need for models that can handle such uncertainty. In this talk, we derive a microstructural, hyperelastic model for transversely isotropic soft tissues and use it to model the mechanical behaviour of tendons. To account for parameter uncertainty, we employ a Bayesian approach and apply an adaptive Markov chain Monte Carlo algorithm to determine posterior probability distributions for the model parameters. The obtained posterior distributions are consistent with parameter measurements previously reported and enable us to quantify the uncertainty in their values for each tendon sample that was modelled. This approach could serve as a prototype for quantifying parameter uncertainty in other soft tissues. Keywords: hyperelastic microstructural tendon modelling; fibrous soft tissues; Bayesian statistics; Random Walk Metropolis Markov Chain Monte Carlo

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Lightning Laplace solvers for free-surface problems

Edward Hinton
University of Melbourne
Peter Baddoo, MIT

Recently, the "lightning Laplace solver" has been proposed for solving Laplace's equation on fixed domains with corners (Gopal and Trefethen, 2019). The lightning solver represents the solution as a rational function whose coefficients are determined by least-squares fitting on the boundary. Root-exponential convergence of the scheme is guaranteed by clustering poles exponentially close to the corners of the domain. However, previous versions of the solver are only applicable to fixed domains where the domain boundary is known in advance. In this talk, we introduce a lightning Laplace solver for free-surface problems in which the domain boundary is unknown and may evolve in time. Such problems are ubiquitous in porous media flows, Hele-Shaw cells, phase transition and many other contexts. We develop an algorithm in which the free-surface is updated at each time step in accordance with the kinematic boundary condition. Unlike the traditional lighting method, we place poles adaptively based on local properties of the boundary. The solutions are obtained significantly faster than traditional numerical methods and enable accurate computation of cusps. Examples are presented for a variety of problems including porous gravity currents and two-phase stable and unstable flows in Hele-Shaw cells.
Keywords: Applied complex analysis, free-surface flows, numerical methods

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Theoretical estimates of the parameters of longitudinal undular bores in PMMA bars based on their measured initial speeds

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K.R. Khusnutdinova (Loughborough University), J.M. Huntley (Loughborough University), P.D. Ruiz (Loughborough University)

We study the evolution of the longitudinal release wave that is generated by induced tensile fracture as it propagates through solid Polymethylemethacrylate (PMMA) bars of different constant rectangular cross section [1, 2]. The wave is measured using high speed single point and multi-point photoelasticity. In all cases, oscillations develop at the bottom of the release wave which exhibit the qualitative features of an undular bore. The viscoelastic extended Korteweg - de Vries (veKdV) equation describes the bore well for a suitable choice of fitted parameters, whilst the analytical solution to the linearised near pre-strain Gardner equation can describe the first oscillation of the bore. From the experimental wave speed and strain rate measured close to the fracture site, we use the analytical solution to obtain estimates for the evolution of the bore at a further distance. The estimates are then compared to corresponding experimental measurements where good agreements are established [2]. References:

[1] C.G. Hooper, P.D. Ruiz, J.M. Huntley, K.R. Khusnutdinova, Undular bores generated by fracture, Phys. Rev. E 104, 044207 (2021). [1] C.G. Hooper, K.R. Khusnutdinova, J.M. Huntley, P.D. Ruiz, Theoretical estimates of the parameters of longitudinal undular bores in PMMA bars based on their measured initial speeds, arXiv: 2110.11843 [nlin.PS] 22 Oct 2021. Keywords: Fracture, Undular Bore, Pre-strain, Viscoelastic

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A Thermal Single Particle Model with electrolyte(TSPMe)

Mat Hunt

University of Warwick

Ferran Brosa Planella (University of Warwick), Florian Theil (University of Warwick), Dhammika Widanalage (University of Warwick)

With the rise of renewable intermittent energy and electric vehicles(EVs), there has been a corresponding requirement for energy storage - batteries. In the early 1990's a comprehensive mathematical model was put forward by Doyle, Fuller and Newman which provided very good predictions for the discharge of the lithium-ion battery but was only for fixed temperature. Industry has been driving fast charge times which necessarily implies a large temperature change.

In this talk, we will use asymptotic reduction on a model by Hunt, Brosa Plannella, Theil and Widanalage to reduce a three scale model for the temperature distribution of a cylindrical battery down to one in only 2 scales. The inclusion of a current density throughout the battery allows us to have varied lithium concentrations in the electrode particles which is more than the usual Single Particle Model(SPM) which is assumed the same throughout the battery. Another result from our analysis is that Joule heating is small in comparison to reversible and irreversible heating. Keywords: Asymototic analysis; lithium-ion batteries; thermal response

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Nonlinear Oscillations of Levitated Air Bubbles

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The oscillations of bubbles play a crucial role in several important physical processes, such as the collapse of cavitation bubbles and the radiation of light via sonoluminescence. Experimental results will be presented that validate the analytical model of Tsamopoulos and Brown (1983) for nonlinear shape oscillations of bubbles. A novel levitation technique has been used to observe the nonlinear oscillations of a

levitated air bubble in water using a high-speed camera. Large axisymmetric perturbations are initially introduced to the system via bubble coalescence. Numerical simulations were carried out using the open source multiphase Navier-Stokes volume of fluid solver Basilisk. A quadratic relationship between frequency and amplitude is found, and mode coupling is observed as predicted by the analytical model of Tsamopoulos and Brown. Good agreement is found between experiment, numerical simulation, and the analytical model.

Tsamopoulos, J., & Brown, R. (1983). Nonlinear oscillations of inviscid drops and bubbles. Journal of Fluid Mechanics, 127, 519-537. doi:10.1017/S0022112083002864

Keywords: bubbles, nonlinear oscillation, multiphase flow

Optimisation using delay-induced bifurcations

Natalia B. Janson
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Finding the best solution, called optimisation, mathematically amounts to finding the global minimum of some cost function. Traditionally, optimisation has been automated with digital or quantum computers, each having their limitations and none guaranteeing an optimal solution. Here, we conceive a novel principle behind optimisation based on delay-induced bifurcations in nonlinear systems with time delay. This could potentially be implemented in analogue devices and lead to optimising machines faster than digital, and cheaper than quantum computers.

Popular optimisation approaches are often interpreted via a particle moving in a multi-well energy landscape. To prevent confinement to a local minimum and to prompt the search for the global one, mechanisms are needed to overcome barriers between the minima. Simulated annealing digitally emulates pushing the particle over a barrier by random forces and requires algorithmic decision-making at every step, which slows down optimisation process. Quantum computers utilise quantum tunnelling through barriers, are technologically challenging and very expensive.

We propose to enable the system to explore all available minima spontaneously, i.e. without the need for continual decision-making, by replacing random forces with dynamical chaos [1]. However, an expectation that chaos occurs reliably and has predictable properties for all energy landscapes might seem inconsistent with nonlinear systems being highly sensitive to the specifics of the equations and generally unpredictable.

To predictably generate global chaos, we utilise a time delay. This might seem counter-intuitive, since normally introducing a delay into a non-linear system makes an already complex situation even more complex. However, we hypothesize and verify that for a certain broad class of the systems with delay, an increase of the delay consistently leads to a sequence of global bifurcations and then global chaos. Such systems can be obtained by taking a standard gradient dynamical system and replacing the argument of its right-hand side with a delayed state variable. A sufficiently large delay compels the system to visit all minima of the cost function.

The barriers between the minima disappear thanks to homoclinic or heteroclinic bifurcations which reconfigure the manifolds originally separating different attractor basins so that they stop separating them [2]. This first study proves the principle for one-dimensional systems with delay.

[1] N.B. Janson and C.J. Marsden, Optimization with delay-induced bifurcations, Chaos 31, 113126 (2021) https://doi.org/10.1063/5.0058087

[2] N.B. Janson and C.J. Marsden, Delay-induced homoclinic bifurcations in modified gradient bistable systems and their relevance to optimization, Chaos 31, 093120 (2021) https://doi.org/10.1063/5.0035959

Keywords: dynamical system, time delay, homoclinic bifurcation, global bifurcation, optimisation

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Travelling wave and asymptotic analysis of a multiphase moving boundary model for engineered tissue growth

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Reuben D. O'Dea and Nabil T. Fadai

The eukaryotic cell cytoskeleton is a complex and evolving network of proteins (mainly actin filaments) that contribute to cell shape, structure, and stability. A cell adheres to a substrate by forming a link between integrins on the cell membrane and ligands in the extra-cellular matrix (ECM). Actin filaments grow into the cell from these links, forming part of the cell cytoskeleton: in this way the cytoskeleton is directly coupled to the ECM. In response to loading, more integrins and mechanically sensitive linker proteins (connecting integrins to the cytoskeleton) are recruited to form mature focal adhesions, in turn promoting expression of signalling proteins which increase actin polymerization and filament cross-linking, leading to the formation and strengthening of contractile actomyosin stress fibres. This process is a pivotal in non-motile cells, where stress fibres are generally of ventral type, interconnecting focal adhesions and producing isometric tension. The strengthened stress fibres then exert a force on the adjoined focal adhesions, closing a feedback loop and leading to overall cell contraction.

We formulate a one-dimensional continuum model to describe this cell-substrate interaction feedback loop, using this model to predict cell contraction and investigate the effects of ligand patterning, inhibitors and collagen remodelling, with the aim to understand how cells respond to external cues in vitro. This model is similar in spirit to some existing models for actin polymerisation in rapidly moving cells. We use a set of reaction-diffusion-advection equations to describe two sets of coupled biochemical events: the polymerization of actin and bundling of the resultant fibres (together with their activation); and the formation and maturation of adhesions between the cell and substrate. The evolution of key proteins is then coupled to a Kelvin-Voigt viscoelastic description of the cell cytoplasm.

The predictions of this model are in line with experimentally observed behaviour with focal adhesion formation near the cell edges and activated ventral stress fibres concentrated towards the cell interior. This model hence constitutes a platform for systematic investigation into how the cell biochemistry and mechanics influence the growth and development of the cell and facilitates prediction of internal cell measurements that are difficult to ascertain experimentally, such as stress distribution. Keywords: Tissue engineering, Reaction-diffusion model, Asymptotic analysis, Travelling waves, Darcy's law

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Crime and neighbourhoods, or how the community's actions affect crime rates

Laura Jones
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What if residents of a neighbourhood could influence crime rates by their behaviour? This is what postulates the theory of collective efficacy. Collective efficacy is the conviction shared by a group of people that they can work together to successfully complete a specific task. The idea is that the difference in neighbourhoods' inner structure leads to spatial variation in crime rates. Many models exist that show the negative link between collective efficacy and crime but the literature in studying the formation of patterns is still limited. We present a novel convolution model of collective efficacy that allows for a mathematical investigation of neighbourhood and resource effects on the formation of collective efficacy and transitions between different regions of collective efficacy. Keywords: criminology; hotspot formation; convolution product; Fourier transform

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Tilings in block copolymers using Strong Segregation Theory

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Daniel J Read and Alastair M Rucklidge (University of Leeds)

Block copolymers can phase separate into different morphologies, influenced by their structure and interactions between component monomers. This feature of block copolymers gives it a designation of designer soft matter where we can find varieties of structures including quasicrystals. It is already well established that phase separated morphologies can be periodic or aperiodic depending upon polymer chain architecture and monomer interactions. Dodecagonal aperiodic tilings were discovered in three-component star block copolymers [1] and understanding the stability of these structures remains an open theoretical question. In our work, we explore whether manipulating the structure and monomer interactions of star block copolymers can lead to phase separation that will self-assemble into quasicrystalline morphologies. Phase separation in block copolymers is studied using three main theoretical frameworks: Weak Segregation Theory (WST), Self-Consistent Field

Theory (SCFT) and Strong Segregation Theory (SST). In SST minimum free energy is calculated from stretching free energy of the polymer chain and interfacial free energy for simple geometrical structures that are formed in phase separation [2,3]. We combine concepts of tiling with SST to examine the stability of periodic and periodic approximants of quasicrystal tilings. The aim is to make experimentally valid predictions of which polymer architectures could lead to stable two- and three-dimensional quasicrystals or other structures.

[1] Kenichi Hayashida, Tomonari Dotera, Atsushi Takano, and Yushu Matsushita. Polymeric Quasicrystal: Mesoscopic Quasicrystalline Tiling in A B C Star Polymers. Physical Review Letters, 98(19) [2] Peter D. Olmsted and Scott T. Milner. Strong segregation theory of bicontinuous phases in block copolymers. Macromolecules, 31(12):4011 4022, 1998 [3] Tohru Gemma, Akira Hatano, and Tomonari Dotera. Monte Carlo simulations of the morphology of ABC star polymers using the diagonal bond method. Macromolecules, 35(8):32253237, 2002. Keywords: soft matter, polymer, quasicrystal, tilings, self-assembly

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Nutrient Transport in a Fibrous Bioreactor Scaffold

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Sarah Waters (University of Oxford), James Oliver (University of Oxford), Jon Chapman (University of Oxford)

Tendon tissue engineering aims to grow functional tissue for transplantation. Cells are grown in a bioreactor which regulates their biochemical and mechanical environment. One approach under development at the Nuffield Department of Orthopaedics, Rheumatology and Musculoskeletal Sciences grows tendon cells on a bundle of flexible fibres, the bioreactor scaffold, surrounded by nutrient-rich media. The cell-seeded fluid-fibre scaffold is actuated by a robotic shoulder to provide mechanical stimulation to the growing cells. Nutrients are delivered to the growing cells by the flow of media through the scaffold. Motivated by this tendon tissue engineering application, we present homogenisation of the nutrient transport equations within the fibrous scaffold. We exploit the small ratio of the fibre separation to the scaffold width to obtain an effective model describing advective and diffusive transport and cell uptake of nutrient within the fluid-fibre scaffold. A poroelastic model is used for the fluid-fibre construct obtained using homogenisation via multiscale asymptotics. We highlight the relationship between the mode of nutrient transport and the size of the Peclet number relative to the fibre separation. In the richest limit where advection, diffusion and uptake balance in the macroscale equations, we also use multiple scales in time to average over the fast timescale of fibre oscillation which characterises transport on the spatial microscale to obtain the time evolution of the nutrient concentration over the whole scaffold. Solutions to the macroscale problem in a simple geometry will be presented, with a reflection on their implications for the bioreactor application. Keywords: Asymptotic homogenisation, Multiscale Modelling, Porous Media, Tissue Engineering

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The hydrodynamic instability in quadratic sheared flow over acoustic linings

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Jet engines, with increasing noise restrictions, make use of acoustic linings to reduce sound attenuation. Modelling these reduces the engine to a duct and the lining to an impedance boundary condition. Making use of the Fourier transformed Euler equations, one can locate 'wave modes' that act as poles in contribution to Fourier inversion by residues. These wave modes can be located by numerical methods and in many cases include an unstable mode with a growing contribution. Under a sheared flow a branch cut, known as the critical layer, is also present but is often ignored from the Fourier inversion. Solving the problem analytically for a quadratic shear allows us to track the poles as we vary the system parameters and find that the unstable mode may become stable. This occurs by moving the pole moving through the branch cut and onto another Reimann sheet, where numerical methods would no longer be able to locate it. The poles contribution when this occurs is absorbed by the critical layer branch cut, suggesting the critical layer branch cut cannot be ignored. Keywords: Aeroacoustics; Sound waves; Complex Analysis; Duct Acoustics

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The Local Anisotropic Basis Function method - a mesh-free framework for high-order DNS in complex geometries

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In the context of direct numerical simulations, the consistency and convergence characteristics of a method are of fundamental importance. The twin requirements of a high degree of accuracy and efficiency have left finite difference and pseudo-spectral schemes to dominate the field. Whilst high-order unstructured mesh methods are possible, for complex geometries, the generation of a quality mesh can be extremely time consuming. Mesh-free methods largely obviate the difficulties of domain discretisation - the process is fast and easily automated. However, most mesh-free schemes (e.g. Smoothed Particle Hydrodynamics (SPH)) are of low accuracy. High-order mesh-free schemes are highly desirable.

Here we present the Local Anisotropic Basis Function Method (LABFM). LABFM enables the efficient calculation of high order derivative operators on an unstructured node discretisation, by solving local consistency matrices such that errors below a certain order are eliminated on a node-by-node basis. Spatially varying resolution is handled naturally, and there is significant potential for schemes with adaptivity of resolution and accuracy (akin to hp-adaptivity). In specific circumstances, LABFM

can be made to collapse to SPH in the low order limit, though LABFM generally differs from high-order consistency corrections to SPH through careful construction of its basis functions which, for example, may incorporate classical orthogonal polynomials. An extremely high order scheme is achieved, with accuracy, consistency and stability properties akin to high order finite differences but with applicability in complex geometries.

We simulations of the fully compressible Navier-Stokes equations, showing up to 10th order consistency and 9th order convergence. With a robust characteristic-based boundary condition framework in place, we conduct simulations in complex geometries with 4th order accurate boundary conditions and a 6th order accurate discretisation internally. Our results also highlight the potential of the method for variable resolution, with simulations containing multiple orders of magnitude of resolution refinement, allowing resources to be focused more efficiently. In an Eulerian framework, LABFM is competitive with leading mesh-based methods, providing the accuracy and efficiency of high-order finite differences, and greater geometric flexibility than unstructured mesh-methods. Keywords: numerical methods, mesh-free methods, high-order, complex geometries, porous media, direct numerical simulation, turbulence

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Nemtsov's Problem

Oleg Kirillov

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We consider a problem of stability of a membrane of an infinite span and a finite chord length, submerged in a uniform flow of finite depth with free surface. In the shallow water approximation, Nemtsov (1985) has shown that an infinite-chord membrane is susceptible to flutter instability due to excitation of long gravity waves on the free surface if the velocity of the flow exceeds the phase velocity of the waves and related this phenomenon with the anomalous Doppler effect. In the present work we derive a full nonlinear eigenvalue problem for an integro-differential equation for the finite-chord Nemtsov membrane in the finite-depth flow. In the shallow- and deep water limits we develop a perturbation theory in the small added mass ratio parameter acting as an effective dissipation, to find explicit analytical expressions for the frequencies and the growth rates of the membrane modes coupled to the surface waves. We find an intricate pattern of instability pockets in the parameter space and describe it analytically. The case of an arbitrary depth flow with free surface requires numerical solution of a new non-polynomial nonlinear eigenvalue problem. We propose an original approach combining methods of complex analysis and residue calculus, Galerkin discretization, Newton method and parallelization techniques implemented in MATLAB to produce high-accuracy stability diagrams within an unprecedentedly wide range of system's parameters. We believe that the Nemtsov membrane plays the same paradigmatic role for understanding radiation-induced instabilities as the Lamb oscillator coupled to a string has played for understanding radiation damping. Keywords: fluid-structure interaction, water waves, radiation-induced instability, flutter, free surface flow

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Multiscale modelling of cell cytoskeleton rheology

Jakub Koery

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Nick Hill, Xiaoyu Luo and Peter Stewart (University of Glasgow)

Eukaryotic cells exhibit a complicated rheology in response to mechanical stimuli, including an elastic response due to the cell cytoskeleton (a network of cross-linked filamentous proteins) and a viscous response due to transport of cytosol through this network. Rational upscaling of existing detailed (but computationally expensive) discrete models into continuum is largely missing and the manner in which microscale parameters and processes manifest themselves at the macroscale is thus often unclear.

We introduce a discrete mathematical model for the mechanics of the cell cytoskeleton. The model involves an initially regular (planar) array of pre-stretched protein filaments (e.g. actin, vimentin) that exhibit tensile forces and resistance to bending. Assuming that the inter-crosslink distance is much shorter than the region of the cell under consideration, we upscale the force balance equations using discrete-to-continuum methods based on Taylor expansions to form a continuum system of governing equations and infer the corresponding macroscopic stress tensor.

We solve these discrete and continuum models numerically to analyse an imposed displacement of a small bead placed in the domain and infer force-displacement curves, which show good quantitative agreement between the approaches. Furthermore, we linearise the continuum model to derive analytical approximations of the stress and strain fields in the neighbourhood of the moving bead, explicitly computing the net force required to generate a given deformation as a function of model parameters including the bead radius and the filament pre-stress.

Future work will also incorporate nonlinear effects in polymer elasticity and the additional influence of fluid transport within the cytoskeleton. Keywords: mathematical biology, multiscale modelling, cell modelling, pre-stress, semiflexible filaments

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Navier-Stokes equations on a manifold from a non-conservative action principle

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David Tsang and Karsten Matthies (University of Bath)

We derive the equations of motion for a viscous barotropic fluid on a manifold using the non-conservative action principle of Galley (2013). Analogous to Galley, Tsang, Stein (2014), where the viscous isentropic fluid equations were derived in Euclidean space, we vary an action functional of the doubled states. The Lagrangian consists of kinetic energy and potential energy terms for each copy of the states, and a non-conservative potential modeling viscosity which couples the two copies of the states. Making the assumption that the fluid is isotropic and Newtonian, we reproduce the compressible Navier-Stokes equations in a coordinate-free manner.

Keywords: geometric mechanics, fluid dynamics, variational principle

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Diffraction by a Right-Angled No-Contrast Penetrable Wedge Revisited: A Double Wiener-Hopf Approach

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About 60 years ago, Radlow claimed to have found an analytical solution for two important and open wave diffraction problems: diffraction by a penetrable wedge (2D) and diffraction by a quarter-plane (3D). He used an innovative approach based on a double Wiener-Hopf technique. However, his solutions were found to be erroneous as they led to wrong near-field asymptotics. Because Radlow stated his solutions 'out of the blue' and his subsequent proofs were non-constructive, it was difficult to pinpoint exactly where he went wrong.

In this talk, we revisit his innovative approach to the penetrable wedge problem and present a constructive way of obtaining his ansatz. The two-complex-variable Wiener-Hopf equation is reduced to a system of two equations, one of which contains Radlow's ansatz plus some correction term consisting of an explicitly known integral operator applied to a yet unknown function, whereas the other equation, the so called 'compatibility equation', governs the behaviour of this unknown function.

Finally, we discuss potential applications of these novel equations.

Reference: Valentin D. Kunz and Raphael C. Assier. Diffraction by a Right-Angled No-Contrast Penetrable Wedge Revisited: A Double Wiener-Hopf Approach. arXiv, 2112.03173, 2021

Keywords: Wave diffraction, Wiener-Hopf, Penetrable wedge

Analysis of Schwarz algorithms for the modified Euler-Tricomi equation

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In mathematics, the Euler-Tricomi equation is a second-order linear partial differential equation that was introduced by the Italian mathematician Francesco Giacomo Tricomi and it is very useful in the study of transonic flows. More precisely, it is a very useful equation for modeling a particular problem with practical applications. The nature of this equation can be complicated ([7], [8]), but we focus on a simplified version for our analysis. The main goal is to implement and analyze the parallel Schwarz algorithms and obtain weak scalability results for this type of problem [4]. Usually, in complicated problems, the one-level methods are not sufficient and a coarse level correction is required, and this has appeared in various works in the literature. For instance, in elliptic problems such as the Laplacian equation, one-level methods are inadequate and the addition of coarse space is needed. However, under certain circumstances, the one-level methods can be enough. In the case of time harmonic problems and elliptic problems ([1], [2], [3], [5], [6]) there is no need for coarse space when the subdomains have a certain geometry such as rectangles of fixed size. For the case of time harmonic problems, the configuration corresponds to a waveguide problem. In the same spirit, we provide results that one-level methods are scalable when implemented to solve the modified Euler-Tricomi equation. The analysis is done in the two-dimensional case where the domain is a large rectangle decomposed into smaller subdomains of equal size.

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3 "Optimizing transmission conditions for multiple subdomains in the Magnetotelluric Approximation of Maxwell's equations", V.Dolean, M.Gander, A. Kyriakis

4 "Analysis of Schwarz algorithms for the modified Euler-Tricomi equation", in preparation, A. Kyriakis

5 "Closed-form optimized transmission conditions for complex diffusion with many subdomains", V. Dolean, M. Gander, A. Kyriakis

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8 “Tricomi and Generalized Tricomi Equations- EqWorld”

Keywords: Domain decomposition methods, Scalability analysis, Generalized Tricomi equation, transonic flows

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A Quantum Graph Approach to Meta-Material Design

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Over the past 20 years metamaterials have gained a large amount of attention due to their potential for possessing highly nontrivial and exotic properties, such as cloaking or perfect lensing. There has been a great push to create models that accurately describe the required material composition that would yield such properties. In this paper, we will introduce a novel quantum graph approach to metamaterial design. The properties of a metamaterial are investigated through the engineering of the resulting band diagrams, then exemplified by Gaussian beam construction. To showcase the engineered refractive properties, two different meta-surfaces are married together, and the required boundary conditions solved. These equations are then extended to N layered metamaterials and examples are presented to showcase the resulting engineered material properties. The proposed quantum graph technique is very flexible and can be easily adjusted making it an ideal design tool for creating meta-materials with exotic band diagram properties or testing promising multi-layer set ups, for example. Keywords: Meta-Materials; Quantum Graphs; Negative Refraction; Wave Modelling;

Parameter-dependent ordinary differential equation (ODE) model identification of systems having local bifurcation

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Model identification using ordinary differential equations (ODEs) is used extensively in many domains, including for digital twins, and infectious disease modelling. The ODE model identification from measured data is generally a parameter estimation problem of the form

$$\dot{x} = f(x, u, t; \theta) y = \varphi(x, t; \theta),$$

where x is a state variable, u is a time-dependent input, θ is a model parameter vector, y is a measured signal, f defines the vector field, and φ defines the observable. There have been many studies on the above problem, and it is worth noting recent advances that apply machine learning techniques such as universal differential

equations (UDEs) and neural ODEs. However, few studies deal with parameter-dependent ODEs undergoing bifurcations of limit sets, such as equilibrium or periodic orbits. Our main objective is to develop an efficient parameter estimation methodology for these cases. ODEs with bifurcations often have a low-dimensional invariant manifold preserved under the flow. From a physical experiment, we can extract the bifurcation structure on the invariant manifold if we use experimental bifurcation schemes such as control-based continuation (CBC) or delayed feedback control. We use knowledge of the invariant manifold and the bifurcation structure of the limit sets as domain knowledge for the model identification problem. We applied the developed methodology to two real-world experiments. First, an aeroelastic experiment where an aerofoil undergoes flutter in a wind tunnel. Flutter is a self-excited vibration of a wing structure due to Hopf bifurcation, which has a centre manifold near the Hopf bifurcation point. A parameter-dependent ODE model is identified using the results of a CBC experiment, which tracks the branch of periodic solutions emerging from the Hopf bifurcation point. The identified model shows good prediction results. Second, a harmonically forced nonlinear mechanical system with an asymptotically stable equilibrium. This system has an invariant manifold known as a spectral submanifold (SSM) near the equilibrium. The model was built using data from a CBC experiment, and the model accurately captures the frequency-amplitude dependency of resonance.

Keywords: ODE model identification, Invariant manifold, Bifurcation

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Simplicial Effective Resistance and Enumeration of Spanning Trees

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A graph can be regarded as an electrical network in which each edge is a resistor. This point of view relates combinatorial quantities, such as the number of spanning trees, to electrical ones such as effective resistance. The second and third authors have extended the combinatorics/electricity analogy to higher dimension and expressed the simplicial analogue of effective resistance as a ratio of weighted tree enumerators. In this paper, we present a new method to compute simplicial weighted tree enumerators using this combinatorial interpretation for effective resistance. We first apply this method to prove a new enumeration formula for color-shifted complexes, confirming a conjecture by Aalipour and the first author, and generalizing a result of Ehrenborg and van Willigenburg on Ferrers graphs. We then apply it to recover an enumeration formula for shifted complexes, first proved by Klivans and the first and fourth authors. In each case, we give explicit expressions for simplicial effective resistances of added facets by constructing a high-dimensional analogue of currents and voltages (a homological cycle and a cohomological cycle). Keywords: Electrical networks, simplicial networks, combinatorics

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A mathematical model to describe the dynamics and scaling of nuclear growth in discrete cytoplasmic volumes

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Scaling of nuclear size with cell size has been observed in many species and cell types. In this work we formulate a modelling framework based on the limiting component hypothesis. We derive a family of spatio-temporal mathematical models for nuclear size determination based on different transport and growth mechanisms. We then analyse model properties and use in vitro experimental data to identify the most probable mechanism. Our analysis suggests that nuclear volume scales with cell volume and that a nucleus controls its import rate as it grows. We further test the model by comparing to data of early frog development, where rapid cell divisions set the relevant time scales. Keywords: nuclear growth, mathematical biology, PDEs

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Fully developed free surface 2-D flow liquid layer encountering a 3-D hump

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This report investigates the two-dimensional steady flow of a liquid layer over a shallow three-dimensional hump at high Reynolds number. The flow is assumed to be incompressible and laminar, the fluid is assumed to be thin so that the viscosity of the solid surface effect up to the free surface of the fluid. A double-decked structure is used to analyze the problem and the pressure-displacement relation is obtained by the analysis. Linearized solutions for small perturbations are generated by the Fourier-Chebyshev method and some flow properties have been determined, such as the flow direction around the hump, the shape of free surface perturbation, and the impact of surface tension on the free surface perturbation. Solutions of two-dimensional nonlinear problems are generated with different numerical methods, the efficiency and accuracy of these methods were compared. Keywords: boundary layer theory; triple deck theory; numerical algorithms; large scale PDEs

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Control of diffusion-driven pattern formation behind a wave of competency

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In certain biological contexts, such as the plumage patterns of birds and stripes on certain species of fishes, pattern formation takes place behind a so-called "wave of competency". Currently, the effects of a wave of competency on the patterning outcome is not well-understood. In this study, we use Turing's diffusion-driven instability model to study pattern formation behind a wave of competency, under a range of wave speeds. Numerical simulations show that in one spatial dimension a slower wave speed drives a sequence of peak splittings in the pattern, whereas a higher wave speed leads to peak insertions. In two spatial dimensions, we observe stripes that are either perpendicular or parallel to the moving boundary under slow or fast wave speeds, respectively. We argue that there is a correspondence between the one- and two-dimensional phenomena, and pattern formation behind a wave of competency can account for the pattern organization observed in many biological systems. Keywords: Turing pattern, diffusion-driven instability, pattern formation

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Modelling Confined Nanoscale Films

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The study of thinfilms at nanoscale has attracted increasing attention due to their importance for various applications such as high performance lubricant, lab-on-a-chip devices, as well as spin coating and printable electronics. The success of these technologies relys on a precise description of the behaviour of thinfilms at nanoscale, where the random (Brownian) movement of particles begins to play an important role. One interesting experimental observation is the thermal capillary waves, generated by random motions of liquid particles perturbing the free surface. The fluctuating hydrodynamics (the Landau-Lifshtiz Navier-Stokes equations) has been raised to include these random motions when describing fluids and for thinfilms, the stochastic lubrication equation has been derived. Periodic boundary conditions have usually been applied in previous works but this is unphysical in real life and the confinement of thinfilms by boundaries (e.g. solid walls) could be important. In this talk, we present the results of the 2D nanoscale thinfilms $h(x,t)$ with two different physically motivated contact line conditions, where the free surface meets a confining wall. To understand the behaviour of the film, we run Molecular Dynamics (MD) simulations and rationalise the results of these using conventional mathematical techniques applied to the stochastic lubrication equation. A linear stability analysis provides information of the wave modes expected for different boundary conditions and generates results that agree excellently with the MD. These results show the

importance of including confining boundaries, even for relatively long films, and we conclude with ideas as to how these results can be experimentally validated. Keywords: Nanofluidics, Free Surface Flows, Thermal Capillary Waves

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Averaged interface conditions: evaporation fronts in porous media

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Homogenisation methods are widely used to derive averaged PDE models for processes occurring on multiple lengthscales. For scenarios in which processes at interfaces are crucial to the overall system, the effect of these multi-scale processes on the interface conditions also merits investigation. In this talk we show how averaged interface conditions can be derived using combined homogenisation methods and boundary layer analysis. We look at two problems in porous media where the interface effects are particularly important: the chemical cleaning of a contaminated porous material, and evaporation within a porous material. In each case we find both the homogenised PDEs and averaged interface conditions, with the microscale effects included via effective parameters. We use the resulting framework to demonstrate the importance of the microscale interface processes on the motion of the evaporating or reacting front and discuss the implications this has for real-world problems. Keywords: homogenisation, boundary layer analysis, fluid flow and diffusion in porous media, chemical reactions, evaporation

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Highly oscillatory quadrature and low-regularity integrators for nonlinear evolution equations

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Arieh Iserles (University of Cambridge), Nigel Peake (University of Cambridge), Katharina Schratz (Sorbonne University)

Highly oscillatory integrals arise in a plethora of numerical methods for the simulation of physical systems, including in wave scattering and quantum physics. This has motivated a tremendous effort over the recent decades to develop efficient numerical methods for the approximation of such highly oscillatory integrals. Amongst them are so-called Filon methods, which combine ideas from classical quadrature with asymptotic theory to approximate these integrals reliably accurately and at uniform cost in frequency. However, one of the central difficulties encountered in Filon methods is the fast computation of the quadrature moments.

In this talk, we will describe a novel approach to the solution of this 'moment-problem' by providing a general framework for the construction of moment recursions that can achieve this desired task for a wide range of oscillators. In addition, based

on a deep connection between oscillatory phenomena and the regularity (differentiability) of solutions to partial differential equations on periodic domains, we will see how Filon methods can be used in time-stepping methods to accurately capture frequency interactions in nonlinear evolution equations. Based on recent advances in resonance-based integrators, this insight allows us to design innovative numerical schemes, which can efficiently approximate low-regularity solutions to nonlinear systems, even when classical methods (such as exponential integrators) fail. We will see both theoretical results and numerical experiments which demonstrate the favourable performance of the proposed methods. Keywords: Numerical analysis; highly oscillatory phenomena; time-stepping methods; nonlinear partial differential equations

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Dimensions of Level-1 Phylogenetic Networks

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Phylogenetic networks provide a means of describing the evolutionary history of taxa that have undergone “horizontal” events, such as hybridization or lateral gene transfer. The mutation process of a single nucleotide for a set of such taxa can be modelled as a Markov process on a phylogenetic network, and the site-pattern probability distributions from such a model can be viewed as a projective variety. Previous work has shown that level-1 networks under certain group-based evolutionary models are identifiable from their corresponding variety. In recent work, we have been able to describe the dimension of a variety corresponding to a level-1 phylogenetic network under any group-based model of evolution. Our method relies on a simple network decomposition, and methods from tropical geometry. In this talk, I will introduce phylogenetic networks with Markov models of evolution, and their corresponding varieties. I will give an overview of the underlying algebra and describe our results. Keywords: Phylogenetic networks, algebraic statistics, applied algebra

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Extracellular matrix remodelling by neural crest cells provides a robust signal for collective migration

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Neural crest cells (NCCs) exhibit highly invasive phenotypes in vertebrates; they migrate from the neural tube of an embryo throughout its developing tissues. Since many NCC progenitors contribute to homeostasis in mature organisms, it is unsurprising that disruptions to NCC migration can have severe consequences on individual health, ranging from developmental defects to embryonic lethality. However, the relative importance of the biological mechanisms that contribute to the emergence and maintenance of NCC migration patterns remains to be established. Here, we model discrete NCC migratory streams using experimental data in the chick embryo. In collaboration with developmental biologists, we create a new agent-based model (ABM) for NCC migration that examines how remodelling of the extracellular matrix (ECM) can provide a non-local signal that allows cells to maintain coherent streams. We perform a global sensitivity analysis to identify model mechanisms that most contribute to successful migration, and use the ABM to generate in silico predictions to test through in vivo experiments. We find that ECM remodelling, haptotaxis, and contact guidance provide sufficient signals for NCCs to establish robust streams in silico; however, additional mechanisms are required to steer cells towards appropriate target sites. Keywords: collective cell migration, neural crest, extracellular matrix, agent-based modelling, leader-follower migration

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The effect of an electric field on coating flow on the outer surface of a rotating horizontal circular cylinder

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Alexander W. Wray and Stephen K. Wilson (University of Strathclyde)

The dynamics of a thick, two-dimensional film of an electrified, perfectly conducting, Newtonian fluid flowing on the outer surface of a rotating, horizontal, circular cylinder are studied. The rotating cylinder is an electrode held at a constant potential and a concentric outer electrode encloses the system, inducing electrostatic forces at the interface. The potential at the outer electrode is, in general, non-uniform, and its spatial distribution can be prescribed. The long-wave approximation is used along with the Method of Weighted Residuals to derive a model that incorporates the effects of the electric stress, rotation, gravity, viscosity, inertia, and capillarity. This model is investigated both numerically and analytically in appropriate limits. In particular, the model is investigated in detail in the thin-film limit. The cases in which the inner electrode is stationary and rotating with a constant angular velocity are both considered. In the former case, draining is observed, and the behaviour is found to exhibit a common structure across all parameters. Analytical and asymptotic solutions along with scaling laws for the film evolution at late times are derived and validated against numerical simulations of the governing equation. In the latter case, a nonlinear parametric study is performed which identifies four characteristic behaviours of the system: transient behaviour, steady states, periodic states, and outer contact (in which the film comes into contact with the outer electrode), and corresponding parameter planes are determined. In addition, the linear stability of the system is investigated in two analytically-tractable cases, and it is shown that the electric field has an overall destabilising effect on the system. Finally, the thick-film model is used to briefly explore the possibility of controlling the film using the electric field. Keywords: Fluid mechanics; electrohydrodynamics; long-wave; thick-film; thin-film; coating flow

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Improved calculations of waterfalls and weir flows

Elle Mclean

UCL

R. Bowles, B. Scheichl and J.-M. Vanden-Broeck

There have been many studies on two-dimensional free-surface flow over the edge of a plate, forming a waterfall under the influence of gravity, and with uniform horizontal flow far upstream. The assumptions taken are such that we have potential flow. In particular, Dias and Tuck (1991) present numerical solutions for supercritical flows that have been computed using conformal mappings and a series truncation and collocation method. We present an extension to this work where a more appropriate expression is taken for the assumed form of the complex velocity. The justification of this lies in the behaviour of the flow far downstream and the wish to better encapsulate the parabolic nature of such a free-falling jet. New numerical results will be presented, demonstrating the improved shape of the new free-surface profiles. These numerical solutions will also be validated through comparisons with asymptotic solutions, in particular for flows with larger Froude numbers. For flows with Froude numbers closer to 1, we demonstrate that the revised complex velocity ansatz should be employed in place of the asymptotic solution. The revision of the assumed form of the complex velocity is also applied to other similar flows that still involve uniform horizontal flow upstream and the falling jet downstream. Improvements to the jet shape can again be observed. Keywords: Free surface flows

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Surfactant driven cavity flow and contact line singularities

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We model the advective Marangoni spreading of insoluble surfactant at the free surface of a viscous fluid that is confined within a two-dimensional rectangular cavity. This is a fundamental problem similar to the shear or lid-driven cavity flows, with applications for confined surface flows where surfactant can be naturally present, such as for unsteady flows over superhydrophobic surfaces in normal environmental conditions, or artificially added, such as in cleaning problems. Interfacial deflections are assumed small, with triple-phase contact lines pinned to the walls of the cavity; inertia and surface diffusion are neglected. Linearising the surfactant transport equation about the equilibrium state allows a modal decomposition of the dynamics, with eigenvalues corresponding to decay rates of perturbations. Computation of the family of mutually orthogonal two-dimensional eigenfunctions reveals singular flow structures near each contact line, resulting in spatially oscillatory patterns of wall shear stress and a pressure field that diverges logarithmically. These singularities of a stationary contact line are associated with dynamic compression of the surfactant monolayer, but can be regularized by surface diffusion. They highlight the need for careful treatment in computations involving unsteady surfactant transport dominated by advection in confined domains. Keywords: Surfactants, Contact lines, Marangoni.

Ventral stress formation and contraction in cell-substrate adhesion

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The eukaryotic cell cytoskeleton is a complex and evolving network of proteins (mainly actin filaments) that contribute to cell shape, structure, and stability. A cell adheres to a substrate by forming a link between integrins on the cell membrane and ligands in the extra-cellular matrix (ECM). Actin filaments grow into the cell from these links, forming part of the cell cytoskeleton: in this way the cytoskeleton is directly coupled to the ECM. In response to loading, more integrins and mechanically sensitive linker proteins (connecting integrins to the cytoskeleton) are recruited to form mature focal adhesions, in turn promoting expression of signalling proteins which increase actin polymerization and filament cross-linking, leading to the formation and strengthening of contractile actomyosin stress fibres. This process is a pivotal in non-motile cells, where stress fibres are generally of ventral type, interconnecting focal adhesions and producing isometric tension. The strengthened stress fibres then exert a force on the adjoined focal adhesions, closing a feedback loop and leading to overall cell contraction.

We formulate a one-dimensional continuum model to describe this cell-substrate interaction feedback loop, using this model to predict cell contraction and investigate the effects of ligand patterning, inhibitors and collagen remodelling, with the aim to understand how cells respond to external cues in vitro. This model is similar in spirit to some existing models for actin polymerisation in rapidly moving cells. We use a set of reaction-diffusion-advection equations to describe two sets of coupled biochemical events: the polymerization of actin and bundling of the resultant fibres (together with their activation); and the formation and maturation of adhesions between the cell and substrate. The evolution of key proteins is then coupled to a Kelvin-Voigt viscoelastic description of the cell cytoplasm.

The predictions of this model are in line with experimentally observed behaviour with focal adhesion formation near the cell edges and activated ventral stress fibres concentrated towards the cell interior. This model hence constitutes a platform for systematic investigation into how the cell biochemistry and mechanics influence the growth and development of the cell and facilitates prediction of internal cell measurements that are difficult to ascertain experimentally, such as stress distribution.
Keywords: mathematical biology, cell modelling, cell signalling

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A particle level model for a concept silicon reactor

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Traditional refining of silicon leads to carbon monoxide and carbon dioxide emissions into the atmosphere. Instead of lump quartz and carbon, an alternate process uses quartz particles coated in a thin layer of porous carbon as the raw material. This concept reactor operates at a lower temperature, and different chemical reactions occur, reducing the greenhouse gas emissions. As the quartz core is consumed, a void is formed between the quartz and the porous carbon layer. We develop a paradigm model for chemical and transfer processes within a single quartz-carbon pellet. We derive governing equations for the concentration of carbon monoxide and carbon, and conservation equations on the moving quartz interface. We non-dimensionalize our model and reduce to a dilute, distinguished limit. The resulting equations are then solved numerically. We show the time evolution of the concentrations, and how the quartz consumption is affected by varying the parameters of the model.
Keywords: Multi-component gas dynamics, moving interface, porous media

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Evolution of and deposition from an evaporating sessile annular droplet

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H.-M. D'Ambrosio, University of Strathclyde. S. K. Wilson, University of Strathclyde. A. W. Wray, University of Strathclyde. B. R. Duffy, University of Strathclyde. K. Sefiane, University of Edinburgh.

The vast majority of previous work on evaporating sessile droplets has focused on the case of an axisymmetric droplet with a single, circular contact line. In the present work, we formulate and analyse a mathematical model for the evaporation of an axisymmetric annular droplet with two circular contact lines. Not only is the evaporation of annular droplets of intrinsic scientific interest in its own right, but it also arises in several practical and industrial contexts, such as the evaporation of a droplet in a well, which occurs in the manufacturing of organic light-emitting diode (OLED) displays (see, for example, D'Ambrosio et al. [1]). More generally, the evaporation of, and deposition from, droplets other than a single, circular contact line has been the subject of recent interest [2]. Approximate, asymptotic and numerical solutions of the problem for the concentration of vapour in the atmosphere are described and used to determine the local, and hence the global, evaporative flux from the droplet in the diffusion-limited regime. The evolution, and therefore the lifetime, of the droplet in various modes of evaporation, as well as the nature of the deposit left behind on the substrate after the droplet has entirely evaporated, are described both in the diffusion-limited regime and in the special case of a spatially uniform evaporative flux.

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Generator aggregation and power grid stability

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With the increased penetration of intermittent and low-inertia power sources (e.g., solar and wind), greater consideration needs to be given to frequency stabilisation of power grids. One way of doing this is to tune the level of damping in different generators to ensure the best power grid stability; mathematically, this corresponds to choosing a set of damping parameters to minimise the Lyapunov exponent of the coupled system of swing equations representing the grid as a network of effective generators. Previous analysis has shown that choosing different damping parameters for different generation nodes can improve overall stability. However, many grid models aggregate distinct generators together into individual nodes. In this talk, I will show that using existing methods on networks of aggregated generators can seriously undermine the stability gains proposed, and that it is likely that these methods are only useful when each node represents a single generator. Keywords: Power grid; Steady-state stability; Aggregation; Synchronisation

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On the progress of q-fractional differential operators and their applications.

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Olivia Ada Obi

Roughly speaking, the q-calculus can be considered as a calculus without the limits. This modification on the concept of limit makes many applications in different mathematical area such as combinatorics, number theory, basic hypergeometric functions, etc. However, q-calculus faces many restrictions such as losing the symmetry and refusing the chain rule in derivative. One challenges in this area is defining the q-Hadamard operators which has a logarithmic function in its kernel. We remedy the situation by applying different functions in Cauchy iterated q-integral. The result characterizes the new (p,q)-series and leads to new q-fractional differential operators. The applications of this operator in developing q-fractional difference equations are investigated. Besides, the q-calculus discretizes the fractional operator and obtains the new methods of approximation for fractional operators which has been used in different fields of applied mathematics. Keywords: q-calculus, q-fractional differential operators, q-Hadamard operators, q-difference equations

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Slender active loops

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Phoretic microswimmers are typically simply-connected particles (spheres, rods, disks), partially coated in a catalyst, that drive propulsive flows by self-generating local concentration gradients in a surrounding solute. Recently, 3D nanofabrication techniques have enabled the creation of phoretic tori, which exhibit interesting dynamic behaviours. Existing theory for non-simply connected phoretic microswimmers is limited to series expansions for the case of an axisymmetric torus. In this paper, we extend our recent slender phoretic theory to model looped slender filaments of arbitrary 3D centreline, cross-sectional radius, and activity profile. For axisymmetric activity, as in the unlooped case, first-order azimuthal variations in concentration have a leading-order effect on the dynamics. We use our theory to derive analytical formulae for the equivalent stresslet of a uniformly active torus, and the swimming velocity of an axisymmetric "glazed" (Janus) donut. We finally demonstrate the flexibility of the theory by considering deformed tori with non-constant cross-section, and the trefoil knot. Keywords: Microscale flows, locomotion, microbots, diffusiophoresis

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Analytic framework for the flood estimation methods intercomparison

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One of the key problems in flood estimation is to predict the flow in the river after an intensive rainfall. Hydrologists use a variety of methods for such predictions, ranging from physical (PDE) to conceptual to statistical models. These models are often based on different assumptions; such assumptions may be subtle and hidden, and perhaps contradictory.

During the talk I am going to give on overview of our work in systematically developing a rigorous mathematical framework in order to better understand the relations between different classes of models. We develop simple benchmark scenarios for coupled surface-subsurface flows. Extensive data analysis of UK catchments allow for estimation of key non-dimensional quantities. The subsequent study of these models using asymptotic analysis allows us to compare their behaviours in certain limiting scenarios and extract key factors affecting the formation of peak flows.

This intercomparison of asymptotic behaviour of different classes of models can be used as a complementary tool to computational methods for assessing flood model accuracy, and can be used to better understand their applicability limits. Keywords: fluid mechanics, flood estimation, environmental mathematics, asymptotic methods

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Reaction dynamics and early-time behaviour of chemical decontamination

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When a hazardous chemical soaks into a porous material such as a concrete floor, it can be difficult to remove. One approach is chemical decontamination, where a cleanser is added to react with and neutralize the contaminating agent. The goal of this talk is to investigate the reaction dynamics and the factors that affect the efficacy of the decontamination procedure. We consider a one-dimensional porous medium initially saturated with an oil-based agent. An aqueous cleanser is applied at the surface, so the two chemicals are immiscible and a boundary forms between them. A neutralising reaction takes place at this boundary in which cleanser and agent are consumed and reaction products are created. This is a Stefan problem, and the boundary between the cleanser and agent moves as the reaction proceeds. Reaction products formed at the interface may dissolve in one or both liquids. This may temporarily prevent cleanser and/or agent from reaching the reaction site, so diffusion of the chemical species plays a key role. The scenario described above was considered previously by [1] in the limit where the depth of the porous medium is large compared to the length scale over which concentrations vary inside the medium. Here, we present an alternative approach in which the ratio between these length scales can be varied. We will investigate how removal times and reaction dynamics vary with changes in this ratio. We will also discuss and present some results for the early-time behaviour of the system, highlighting the emergence of a boundary layer associated with diffusion in the oil phase similar to that discussed in [2] where the thickness of the boundary layer is directly proportional to the square root of the time variable. [1] M. Dalwadi, D. O'Kiely, S. Thomson, T. Khaleque, and C. Hall. Mathematical modelling of chemical agent removal by reaction with an immiscible cleanser. SIAM Journal on Applied Mathematics, 77(6):1937-1961, Nov. 2017 [2] M. Assuno, M. Vynnycky, S. L. Mitchell. On small-time similarity-solution behaviour in the solidification shrinkage of binary alloys. Eur. J. Appl. Maths, 32:199-225, 2021.

Keywords: Decontamination, Stefan problem

Solving differential equations using neural networks

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Use of neural networks has led to revolutionary progress is the field of machine learning and artificial intelligence. From mathematics viewpoint, neural networks are universal function approximators: a feedforward network with a single layer can approximate any continuous function on a compact set. With the help of optimization schemes, neural networks can be used to approximate solutions of any type of differential equations with several advantages, including speed, memory efficiency and most importantly the ability to generalize to new values in the relevant domain. We present results of several standard differential equations, including 2 and 3 dimensional Bratu-Gelfand equation, Troesch's equation and others.

Modelling high-speed droplet impact onto an elastic membrane

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James M. Oliver (University of Oxford), Matthew R. Moore (University of Hull), Radu Cimpeanu (University of Warwick)

The impact of a high-speed droplet onto an elastic membrane is a highly nonlinear process and poses a formidable modelling challenge due to both the multi-scale nature of the flow and the fluid-structure interaction between the droplet and the membrane. We present two modelling approaches for droplet impact onto elastic membranes: matched asymptotics and direct numerical simulations (DNS). Inviscid Wagner theory is used in the former to derive analytical expressions which approximate the behaviour of the droplet during the early stages of impact, utilising the composite expansion for the pressure to force the membrane. The DNS builds on the open-source volume-of-fluid code Basilisk, with the fluid-structure interaction resolved by changing to a dynamic coordinate system, negating the need to embed a moving boundary into the domain. We show how the speed the droplet spreads across the substrate is notably decreased when the membrane is more compliant, which is consistent with experimental findings that splashing can be inhibited by impacting onto a soft substrate. We conclude by showing how the two modelling approaches are complementary, as a combination of both can lead to a thorough understanding of the droplet impact across timescales. Keywords: Droplets, impact, asymptotic analysis, direct numerical simulations, fluid-structure interaction, free-surface flows

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Averaging and passage through resonances in two-frequency systems near separatrices

Anatoly Neishtadt
Loughborough University
Alexey Okunev

The averaging method is a classical powerful tool in perturbation theory of dynamical systems. There are two major obstacles to applying the averaging method, resonances and separatrices. In this talk we present realistic asymptotic estimates that justify the use of averaging method in a generic situation where both these obstacles are present at the same time, passage through a separatrix for time-periodic perturbations of one-frequency Hamiltonian systems. As a general phenomenon, resonances accumulate at separatrices. The Hamiltonian depends on a parameter that slowly changes for the perturbed system (so slow-fast Hamiltonian systems with two and a half degrees of freedom are included in our class). Our results can also be applied to perturbations of generic two-frequency integrable systems near separatrices, as they can be reduced to periodic perturbations of one-frequency systems.
Keywords: asymptotic analysis

The deformations of fluid conveying elastic-walled tubes

Daniel Netherwood
University of East Anglia
Dr Robert Whittaker

We present a theoretical description of the fluid-structure interaction observed in the Starling Resistor. The typical set-up consists of a pre-stretched finite length thin-walled elastic tube mounted between two rigid sections. The set-up is enclosed within a pressure chamber and a viscous fluid is driven through the system by imposing an axial volume flux. Valid within a long-wavelength thin-walled regime, we use our own results to model the wall motion, which arise from the solution of a generalised eigenvalue problem, and avoids the need to invoke ad-hoc assumptions made in previous studies. The wall mechanics are then coupled to the fluid mechanics using the Navier-Stokes equations, under the assumption that the oscillations in the tube wall are of small amplitude, long-wavelength and high-frequency. We derive the respective steady and oscillatory problems for this fluid-structure interaction. In either case, we compute series solutions, allowing us to calculate the errors incurred after truncation. Keywords: Fluid-structure interaction, Asymptotic analysis, elastic-walled tubes

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Understanding Sensory Induced Hallucinations

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University of Nottingham

Abigail Cocks, Stephen Coombes, Alan Johnston (University of Nottingham) and Daniele Avitabile (VU Amsterdam)

Explorations of visual hallucinations, and in particular those of Billock and Tsou [Neural interactions between flicker-induced self-organized visual hallucinations and physical stimuli. Proceedings of the National Academy of Sciences, 104(20):8490-8495, 2007], show that annular rings with a background flicker can induce visual hallucinations in humans that take the form of radial fan shapes. 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. Here we show that a simple scalar neural field model of primary visual cortex with state-dependent spatial forcing is capable of modelling this phenomenon. Moreover, we show that this occurs most robustly when the spatial forcing has a 2:1 resonance with modes that would otherwise be excited by a Turing instability. By utilising a weakly nonlinear multiple-scales analysis we determine the relevant amplitude equations for uncovering the parameter regimes which favour the excitation of patterns orthogonal to sensory drive. In combination with direct numerical simulations, we use this approach to shed further light on the original psychophysical observations of Billock and Tsou. Keywords: Pattern formation; Amplitude equations; Neural field models

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Uptake of small-scale renewable energy generation: can power grid stability and resilience be maintained?

Reuben O'Dea

University of Nottingham

O Smith, E Farcot, K Hopcraft

The contemporary proliferation of small-scale renewable power generation is causing an overhaul in the topology, composition and dynamics of electrical grids. In contrast to traditional infrastructure, these low output and intermittent generators are widely distributed throughout the grid, including at the household level, resulting in a network that is highly distributed, bi-directional and mutable, for example with households adopting the role of consumers or producers of power as daily and seasonable usage and meteorological conditions vary. With renewable production uptake set to continue in line with initiatives such as "net zero" and the Paris agreement, understanding how this increased complexity impacts robustness of operation is a key challenge with implications for both grid control strategies and future smart grid design.

Marrying network architecture and power flow dynamics with fluctuations in renewable generation and consumer demand, informed by PV generation and household consumption data of approximately 5000 households in the London area, we

investigate the dependence of grid susceptibility to cascading failure on its consumer/generator composition and network structure. Thereby we highlight that the drive towards small-scale renewable generation has an unintended downside, making the micro-powergrid susceptible to outages. Moreover, the installation of household battery storage, which is typically optimised for consumer self-sufficiency rather than network performance, does little to ameliorate this resilience problem. Together, these results advocate for the adoption of new network-level control strategies that are optimised for global, rather than local, performance.

Keywords: Networks, Cascades, Power grid modelling

Asymptotic corrections for extensional flow

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Niall Hanevy, Coventry University

Honey falling from a spoon is an example of extensional flow: a long, thin thread of viscous fluid falls with an axial velocity that is uniform across its radius. Extensional flows also occur in glass drawing processes, where sheets and fibres of molten glass are stretched longitudinally. Mathematical models of these processes often exploit their long-and-thin aspect ratios, and the famous Trouton model describes the leading-order one-dimensional behaviour.

In this talk we re-visit the classic problem of fibre drawing, and consider corrections to the leading-order Trouton model. Non-dimensionalized governing equations contain the aspect ratio with even powers only, which could motivate an asymptotic expansion in powers of the aspect ratio squared. However, numerical solutions and the emergence of boundary layers at the sheet ends both suggest that this approach is wrong: the error in the leading-order solution scales linearly with the aspect ratio. We explain the origin of this discrepancy, and present the larger-than-expected corrections.

Keywords: viscous flow; asymptotic analysis; Trouton model

The Study Of Bi-Geometric Fractional Model For The Treatment Of Cancerous Cells Using Radiotherapy

Olivia Ada Obi

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Olivia Ada Obi, Near East University, Cyprus, and Mohammad Mommenzadeh, Near East University, Cyprus.

One of the oldest and best developed method of studying the population of cancerous and healthy cells in struggled tissue is the mathematical modelling of growth with differentiation and mutation of cells. Thus, their population, under the administration of radiation can be simulated by Lotka-Voltera competition model where the coefficients determine the type of cancer. Fractional differentiation implies a meticulous model with more flexible parameters.

Furthermore, studying fractional differential operators on non-Newtonian calculi obtains different types of fractional operators with distinct singularities. Bi-geometric calculus is a famous example of these calculi which is equipped by the Hadamard fractional differential operator. This model reflects the extension of Bi-geometric derivatives to the fractional case with inevitable consequences of removing the singularity of the integration's kernel in the initial values.

The existence and uniqueness are guaranteed by Arzela-Ascoli theorem and Bi-geometric analogue of numerical methods obtain the approximation. Also, the phase space of different models are investigated by applying matlab programme. Keywords: Lotka-Volterra, Bi-Geometric Calculus, Mathematical Biology.

Building blocks for representing the decay of 3D Navier-Stokes flows and their applications

Koji Ohkitani

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For 2D Navier-Stokes flows it has been understood that the late stage of their time evolution is represented by a collection of isolated vortices, so-called Burgers vortices. In this talk we study an analogue of such elementary excitation, or building blocks, for 3D Navier-Stokes flows.

Let $\boldsymbol{\Psi}, \boldsymbol{U}, \boldsymbol{\Omega}$ and $\boldsymbol{X}$ be the dynamically-scaled vector potential, velocity, vorticity and vorticity curl fields. To leading-order approximation (i.e. linearisation) they look as follows, which are actually close to the nonlinear solutions [1]:

$$\boldsymbol{\Psi} = \frac{\boldsymbol{M} \times \boldsymbol{\xi}}{8\pi^{3/2}} J(r),$$

$$\boldsymbol{U} = \frac{\mathrm{erf(r)}}{4\pi r}\left(\boldsymbol{M} - \frac{(\boldsymbol{M}\cdot\boldsymbol{\xi})\boldsymbol{\xi}}{r^2},\right) - \frac{J(r)}{8\pi^{3/2}}\left(\boldsymbol{M} - \frac{3(\boldsymbol{M}\cdot\boldsymbol{\xi})\boldsymbol{\xi}}{r^2}\right),$$

$$\boldsymbol{\Omega} = \frac{\boldsymbol{M} \times \boldsymbol{\xi}}{4\pi^{3/2}} H(r),$$

$$\boldsymbol{X} = \frac{e^{-r^2}}{\pi^{3/2}} \left(\boldsymbol{M} - \frac{(\boldsymbol{M}\cdot\boldsymbol{\xi})\boldsymbol{\xi}}{r^2} \right) - \frac{H(r)}{4\pi^{3/2}} \left(\boldsymbol{M} - \frac{3(\boldsymbol{M}\cdot\boldsymbol{\xi})\boldsymbol{\xi}}{r^2} \right).$$

Here $\boldsymbol{\xi}$ denotes the spatial coordinates in scaled space, $\boldsymbol{M} = \int_{R^3} \boldsymbol{X} d\boldsymbol{\xi}, r = |\boldsymbol{\xi}|$ and

$$H(r) \equiv \frac{\sqrt{\pi}\mathrm{erf}(r) - 2re^{-r^2}}{r^3},$$

$$J(r) \equiv \frac{re^{-r^2} + \sqrt{\pi}\mathrm{erf}(r)\left(r^2 - \frac{1}{2}\right)}{r^3}.$$

We will discuss their spatial structure and implications as to the near-integrability of the Navier-Stokes equations [2].

References
[1] "Self-similar source-type solutions to the three-dimensional Navier-Stokes equations,"
K. Ohkitani & R. Vanon, to appear in *Proc. Roy. Soc. A*, also arXiv:2107.02952.
[2] "Self-similarity in turbulence and its applications,"
K. Ohkitani, to appear in *Phil. Trans. Roy. Soc. A*, also arXiv:2201.04775.
Keywords: Navier-Stokes equations, self-similarity, scale-invariance, source-type solutions

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Age dependent modelling and its application to COVID-19 outbreak

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The contagiousness of COVID-19 disease and the administration of vaccines differ depending on the age of the individual. The age heterogeneity of the populations involved necessitates considering models in age groups with specific susceptibilities, making the prediction problem more difficult. There are basically three age groups of interest, which are respectively 0-19 years, 20-64 years, and >64 years. We proposed a mathematical age-dependent (Susceptible-Infectious-Goneanewsusceptible-Recovered (SIGR)) model for the COVID-19 outbreak and performed some mathematical analysis to demonstrate the solution's positivity, boundedness, stability, existence, and uniqueness. We proved that the basic reproduction number R0 is near the endemic stationary state and we also performed numerical simulations of the model. We discuss the impact of the model's various parameters, particularly vaccination, on epidemic dynamics. We present a novel approach to improving an age-dependent model and its applications to observed data and parameters from epidemiology. Keywords: SIR model; COVID-19; Age dependent modelling; Demographic model; Epidemic model

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Mathematical models of engine ice crystal icing

Timothy Peters

University of Bath

Hui Tang (University of Bath) and Philippe Trinh (University of Bath)

In the last decade, it has been noted that ice crystal icing (ICI) is responsible for more than a hundred observed instances of power loss and engine damage. In this scenario, ice crystals present at high altitudes enter the hot engine core. Despite the high temperatures in the core, the crystals can accrete on the interior surfaces in a partially melted state, and then shed outwards, damaging key components and causing a power loss. Existing knowledge on the mechanism of ice crystal build-up and shedding is extremely limited, although some models have been recently developed.

In this talk, we present some of the preliminary modelling of ice crystal icing, with particular emphasis on the fundamental physics challenges that exist in such formulations. We discuss the role of key non-dimensional quantities such as the Peclet and Stefan numbers, and the resultant numerical solutions under this model. Finally, we discuss recent efforts to formulate more rigorous and accurate dynamical models of thin water-and-ice films that might account for more complex environmental and geometrical conditions of the engine.

Keywords: mathematical modelling, industrial mathematics, fluid mechanics, thin films

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Confirmation Bias Emerges From an Approximation To Bayesian Reasoning

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The University of Warwick and The Alan Turing Institute

Adam Sanborn, The University of Warwick and The Alan Turing Institute; Eugene Malthouse, The University of Warwick; Thomas T Hills, The University of Warwick and The Alan Turing Institute

Confirmation bias is the observed human behaviour of searching for and assimilating information in a way that favours existing beliefs, more so than would be rational. We present a Bayesian model of belief updating that takes into account beliefs about the central hypothesis in question and the reliability of the source of information. An individual's beliefs about the central hypothesis and the source reliability form a Bayesian network, and are updated simultaneously upon receiving data. This rational updating introduces dependencies between beliefs that can quickly grow and overwhelm any realistic limitation on memory space. We present a normative account of human belief updating that considers cognitive limitations by including an independence approximation that approximates Bayesian rationality with much lower memory requirements. We show how this information processing model can generate many confirmation bias type behaviours, specifically biased assimilation, biased evaluation, attitude polarisation, belief perseverance and confirmation bias

in the selection of sources. Keywords: psychology, bayesian networks, cognition, confirmation bias, rational analysis

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The Effects of Compliance on Various Flow Configurations

Ryan Poole

University of Surrey

This presentation investigates the stability of a two-dimensional jet/wake flow when confined by two compliant boundaries, which are modelled as springsupported plates. By considering the basic flow as piecewise-linear profile we derive analytic dispersion relations $D(\alpha, \omega) = 0$, in the form of 4th order polynomials in the wave frequency ω, with transcendental coefficients in the wave number α. We derive these dispersion relations for both varicose and sinuous flows, and we use these dispersion relations to calculate the temporal and absolute instability characteristics of the flow for a range of flow and boundary parameters. Solving the dispersion relations leads to 4 solutions, two hydrodynamicmodes related to the flow, and 2 wall-modes that are a consequence of having non-rigid boundaries. We find the addition of the compliant boundaries leads to additional instabilities unseen in the case when the flow is bounded by rigid walls, this is true for both temporal and absolute instabilities. We find that we are able to suppress and enhance the magnitude of the absolute instabilities by varying the wall parameters, as well as modifying the range of parameter space where an absolute instability exists. Keywords: Fluid dynamics, stability analysis, Absolute Instability, Flexible walls, jets and wakes

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Droplet evaporation on inclined chemical patterns

Marc Pradas

The Open University

Michael Ewetola (UCL), Matthew Haynes (Bader International Study Centre, Queen's University)

The evaporation of droplets on inclined substrates is important for a broad range of applications, including ink-jet printing, surface cooling, and micro-structure assembly. Despite its apparent simplicity, the precise configuration of an evaporating droplet on a solid surface has proven notoriously difficult to predict and control. Here, we study the effect of smooth patterns on a droplet evaporating on an inclined plane. The evaporation is assumed to be quasi-static so that the dynamics of the droplet can be quantified by the equilibrium properties of the system. We first examine the limiting case of small gravity (small Bond number) and perform asymptotic analysis to obtain approximate solutions. For higher Bond numbers we derive exact solutions written in terms of elliptic integrals that can be solved numerically. By studying the stability of these solutions, and how it depends with the droplet size, we perform a bifurcation analysis that shows the emergence of a

hierarchy of bifurcations that strongly depends on the particular underlying chemical pattern. We show in turn that gravity affects the topology of the bifurcation diagrams, reducing the stability regions of the phase space. To understand the droplet dynamics upon evaporation on inclined surfaces, we perform numerical simulations of the Cahn-Hilliard and Navier-Stokes system of equations. We focus on the quasi-static regime, where droplet evaporation is dominated by diffusion into the gas phase, and the density contrast between fluids is taken into account via a Boussinesq approximation. We observe very good agreement between the numerical results and the behaviour predicted by the quasi-static analysis. Our results show that the interplay between a phase change and surface wettability can be exploited to control the motion of droplets on inclined patterned solid surfaces. Keywords: Wetting phenomena, Droplet evaporation, Bifurcation analysis

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Mathematics, the Mind and Alzheimer's disease: Patterns of progression on brain graph

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Travis B. Thompson, Hadrien Oliveri, Alain Goriely; Mathematical Institute, University of Oxford

The world's population demographics are increasingly trending towards the elderly. As a result, dementia, and Alzheimer's disease (AD) in particular, is now one of the leading causes of death, and of economic pressure, across the Western and Asiatic world. Neurodegenerative diseases also present a clear, and present, challenge to modern medicine due to brain delicate in vivo environment and limited insight from the human whole nervous system. Mathematical network models of dementia, such as AD, offer a path forward that can be deployed using the multitude of anatomical brain-graph data from real human patients. Making use of a mathematical model requires the choice of a mechanistic system of equations in addition to choices regarding the construction of the underlying brain graphs on which the equations evolve. In this talk, I address two questions central to the effective mathematical network modeling of AD: How do the mathematical model and the specific choice of brain graph influence the spectrum of realizable AD progression patterns; and can we estimate how AD will progress using only the information derived from the brain connectivity graph? My research demonstrates that an appropriate choice of network mathematical model can provide important insights, and estimates, for the progression of AD and is an indispensable tool in AD research. Keywords: Neurodegenerative disease; Prion-like propagation; Mathematical network model; Pattern of progression; Brain connectivity graph

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Superadiabatic transitions in Single Switch Surface Hopping

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Benjamin Goddard (University of Edinburgh), Adam Kirrander (University of Edinburgh)

The Born-Oppenheimer approximation, commonly used in quantum molecular dynamics, uses the separation of time scales between the heavy nuclei and the light electrons to decouple their dynamics. As a result, the evolution of the nuclei is confined to a particular electronic eigenspace, significantly reducing the complexity of the problem. However, a non-trivial challenge arises when the separation between energy levels (eigenvalues) is ”small” (denoted an avoided crossing) or zero (conical intersection). Here, one has to accurately account for so-called ’non-adiabatic’ transitions between energy levels. This is commonly done through the Landau-Zener transition rate. We propose an alternative transition rate, the Superadiabatic rate, which stems from the results by Goddard et al. on superadiabatic transitions in the presence of an avoided crossing [1]. We incorporate the Superadiabatic rate within the commonly used Probabilistic Single Switch Surface Hopping algorithm [2] and compare the quality of the resulting algorithm to one using the more famous Landau-Zener rate. Whilst the latter gives accurate results for many systems, it deteriorates significantly in regimes such as where the energy gap is relatively large. We demonstrate the greater performance of the Superadiabatic rate on both model and realistic systems.

[1] “Superadiabatic transitions in quantum molecular dynamics”, V. Betz, B. D. Goddard and S. Teufel. P. Roy. Soc. A-Math. Phy., 485, 3553-3580 (2009). [2] “Landau-Zener type surface hopping algorithms”, A. Belyaev, C. Lasser, G. Trigila. J. Chem. Phys. 140, 224108 (2014). Keywords: quantum molecular dynamics; superadiabatic representations; trajectory surface hopping.

Thick non-axisymmetric flow on the exterior of a vertical fibre

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Fluid flow on the exterior of a fibre is a problem that has been the subject of considerable interest and is relevant to a number of industrial processes such as desalination and heat exchange. Flows down a fibre experience instabilities which cause the formation of a variety of beading patterns (Kliakhandler et al., J. Fluid Mech. **429** 2001, 381–390). Existing models have often assumed that the film is thin (Shlang and Sivashinsky, J. de Physique **43** 1982, 459–466) and/or that the flow is axisymmetric (Ruyer-Quil et al., J. Fluid Mech. **603** 2008, 431–462). However, when the film is sufficiently thick and the flow has a sufficiently high Reynolds number, instabilities that break the axisymmetry of the flow are observed. It has been recently shown that these non-axisymmetric instabilities have more predictable dynamics than axisymmetric instabilities (Gabbard and Bostwick, Phys. Rev. Fluids **6** 2021, 034005). This predictability can be beneficial in industry when certain beading patterns (e.g. a regular beading pattern with maximal bead frequency) are desired. To model the non-axisymmetric instabilities we will use a methodology originally developed for Wray et al. (Wray et al., SIAM J. Appl. Math. **77** 2017, 881–904) to develop a model for the flow of a thick film on the exterior of a vertical fibre. We then use linear stability theory to elucidate the dynamics which determine both the stability and the symmetry of the flow, and compare the predictions from our model against those of the full Navier–Stokes equations. Keywords: Linear stability analysis; fibre; coating flow; thick film.

Modelling the Carding of Recycled Carbon Fibre

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Carbon fibre is a very versatile material with applications in many different industries from medical, electronics, marine to space. The demand for carbon fibre composites is increasing yearly and thus the amount of waste carbon fibre is increasing. This waste can be recovered and turned into a material that can be used in industry. The waste carbon fibre can be converted into a nonwoven using a carding process, as in the textile industry. Carding machines consist of a set of toothed rollers of different sizes, moving in different directions and at different velocities, with the aim of producing a web of aligned fibres. In this study, we model the break up of "tows" of fibres in the carding machine by focusing on the interaction between the fibres and the teeth along the carding rollers. We look at how the properties of the teeth, such as number density and angle, and the properties of the fibres fed into the machine, are related to the efficiency with which the tows are broken up. The aim of this work is to create a continuum model of the process, and hence determine the optimal settings to produce a web of individualised fibres. Keywords: industrial mathematics, mathematical modelling, solid mechanics, differential equations

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PDE-constrained optimization for multiscale particle dynamics

Jonna Roden
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There are many industrial and biological processes, such as beer brewing, nano-separation of colloids and bird flocking, which can be described by integro-PDEs. These PDEs describe the dynamics of a 'particle' density within a fluid bath, under the influence of diffusion, external forces, and particle interactions. They often include nonlinear, nonlocal boundary conditions. A key challenge is to optimize these types of processes, which requires tools from PDE-constrained optimization. In this talk I will introduce a numerical method to solve this class of optimal control problems, which combines pseudospectral and spectral element methods with a Newton-Krylov algorithm. This provides a tool for the fast and accurate solution of the resulting optimality systems. In particular, this framework allows for the solution of (integro-)PDE models and optimal control problems on complex domains, which is a crucial feature in accurately describing various (industry) applications. Finally, some examples of current work and future industrial applications will be given. This is joint work with Ben Goddard and John Pearson. Keywords: Dynamic Density Functional Theory, PDE-constrained optimization, spectral element methods, integro-PDEs

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Linear stability of a viscous, rotating droplet

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Matthew Scase, University of Nottingham, John Billingham, University of Nottingham, Barbara Turnbull, University of Nottingham

We consider the effect of rotation on a viscous mass of fluid initially spun up, centred on the axis of rotation of a solid disk, using a macroscopic slip law and a small contact angle approximation to model contact line dynamics. A thin-film equation for the shape of the free surface is derived from the governing equations and boundary conditions within a rotating frame of reference, which we solve for a steady, axisymmetric, hydrostatic free surface profile. The linear stability of the system is then determined showing the stability is dependent on the nondimensional centrifugal and Bond numbers in the absence of both Coriolis effects and inertia. To solve the equations with an $O(1)$ contact angle, we solve the system numerically using the finite element method on a mesh given by the leading order shape of the free surface, subject to nontrivial stress, slip and regularity boundary conditions. At leading order we find that the $L - 2$ norm of the solutions converge like n^{-1} to the exact hydrostatic solutions, where n is the number of vertices on the free surface.

Keywords: Fluid Mechanics, Free surface flows, Rotating flows

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Oscillatory and chaotic dynamics of solitary waves on falling liquid films

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A liquid film flowing down an inclined plane is an example of a convectively unstable open-flow hydrodynamic system with a rich variety of spatiotemporal structures. These films can have many applications especially in engineering scenarios such as desalination plants and chemical reactors, which makes it important to understand and manipulate the behaviour that is exhibited. At the latest stage of the evolution, the film surface is dominated by interacting solitary waves (pulses), which under certain conditions may form bound states, i.e. a group of pulses travelling with the same speed. In this work we quantify the dynamics of oscillatory states that emerge in a two-pulse system as the Reynolds number is increased. We show that there is a transition from damped oscillatory states to a limit cycle through a Hopf bifurcation, which can be described in terms of resonance poles. For groups of more than two pulses we observe the emergence of chaotic dynamics when pulses are sufficiently close to each other. Keywords: Interfacial Flows, Thin Films, Bifurcation Theory.

Rectangle-triangle soft-matter quasicrystals with hexagonal symmetry

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Aperiodic (quasicrystalline) tilings, such as Penrose's tiling, can be built up from e.g. kites and darts, squares and equilateral triangles, rhombi or shield shaped tiles and can have a variety of different symmetries. However, almost all quasicrystals occurring in soft-matter are of the dodecagonal type. Here, we investigate a class of aperiodic tilings with hexagonal symmetry that are based on rectangles and two types of equilateral triangles. We show how to design soft-matter systems of particles interacting via pair potentials containing two length-scales that form aperiodic (meta)stable states that correspond to two different examples of rectangle–triangle tilings. One of these is the bronze-mean tiling, while the other is a generalization. Our work points to how more general (beyond dodecagonal) quasicrystals can be designed in soft-matter. Keywords: quasicrystals, pattern formation, aperiodic tilings

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Heat spreaders and thermal metamaterials

Eleanor Russell
University of Manchester

Transformation thermodynamics (TT) is an established process for the design of enhanced materials, referred to as thermal metamaterials. To date, TT has been employed to tackle traditional heat transfer problems, with concepts such as thermal concentrators, lenses and uniform heating devices, as well as new and exciting concepts, such as thermal invisibility cloaks and rotators. This talk will focus on employing TT to design funnel-shaped heat spreaders that act as point-to-plane heat source converters in the context of steady-state thermal conduction. The properties of each spreader help to avoid the formation of hotspots by guiding thermal fields in a spatially uniform manner. As a result, a uniform temperature is achieved across the large, convective surface of each spreader when forced by a small heat source at the base. The required properties, which are obtained through TT and can be strongly anisotropic and inhomogeneous, are accurately approximated by assembling isotropic, homogeneous layers, rendering them realisable.

To improve the model of these designs we incorporate the effects of contact resistance between interfaces by replacing perfect contact conditions with temperature jumps. Consequently, we show that some heat spreader designs are significantly affected by contact resistance - especially when many layers are used to approximate the ideal metamaterial properties. Therefore, we propose a simple, alternative design where the funnel-shaped spreaders are split into two or three isotropic, homogeneous components with at most two interfaces - minimising the effects of contact resistance. For these configurations, which we refer to as "neutral layers", a uniform temperature is achieved across the large convective surface by exploiting the solution to the diffusion equation in this geometry, the results of which are tailored to a specific set of boundary conditions.

Our proof-of-concept designs help to gain insight into the potential control and manipulation of thermal fields with unique and novel arrangements of natural materials. We envisage that in the future, these ideas have the potential to be implemented for the effective removal of heat from electronics - a thermal management problem that remains a significant practical challenge. Keywords: Heat transfer, thermal conduction, transformation theory, metamaterials.

Two process models: a nonsmooth dynamics perspective

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Piece-wise linear (PWL) modelling has many useful applications in engineering, social science, finance, and biology, especially in the context of sleep and neurodynamics. Although, there are many techniques to understand the behaviour of smooth dynamical systems, nonsmooth systems are still relatively unexplored. In this talk, I will consider various kind of two process model described by PWL dynamical systems with oscillatory or constant thresholds; including models of sleep/wake regulation and neuronal firing. I will describe the technique to obtain periodic solutions, the augmentation of Floquet theory necessary to determine stability, and the determination of bifurcations (both smooth and non-smooth). Furthermore, I will show how to construct the Lyapunov exponent of a nonsmooth flow and use this to uncover a more detailed picture of the Arnol'd tongue structure of the models considered. Numerical studies will be presented to illustrate theoretical results.

Keywords: Dynamical systems; Piece-wise linear modelling; Two process model; Sleep; Neurodynamics;

Surface-tension-driven evolution of a viscoplastic liquid coating the interior of a cylindrical tube

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One mechanism for airway closure in the lung is the surface-tension-driven instability of the layer of fluid lining the airway wall. The mechanism is well understood for the case where the airway surface liquid (ASL) is Newtonian. However, mucus, the main component of the ASL, is non-Newtonian and has a yield stress, motivating this study of the surface- tension-driven evolution of a layer of viscoplastic Bingham fluid coating the interior of a cylindrical tube. Two evolution equations for the height of the liquid layer are derived, the first using thin-film theory, the second using long-wave theory which does not assume the layer is thin. Both evolution equations are solved numerically and static solutions of each equation are also computed. Unlike in the Newtonian problem, the initial conditions crucially affect the final shape of a viscoplastic layer after its evolution. We find a critical amplitude of perturbation, which depends on the Bingham number, required to make the layer initially yield. Using thin-film theory, we also calculate the branch of static

solutions with monotonic curvature and predict the large set of initial conditions which all evolve towards it, which we verify using numerical simulation. Overall, we find that increasing the yield stress inhibits the instability, either delaying unstable growth and reducing the final peak height of the layer or suppressing the instability entirely. Furthermore, the critical layer thickness for the instability to occur is increased with larger yield stress. These findings have implications for modelling airway closure, particularly in obstructive conditions such as Cystic Fibrosis where the mucus layer is often thicker and has higher yield stress. Keywords: non-Newtonian fluid dynamics; interfacial flows; surface-tension-driven flow; biological fluids

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Reacting counter-current flow of a binary gas mixture and solids in a silicon furnace

Matthew Shirley

University of Oxford

Matthew Moore (University of Hull), James Oliver (University of Oxford), Colin Please (University of Oxford)

In the industrial production of silicon, the raw materials, quartz and charcoal, are fed into the top of the furnace and move downwards. As they are heated up, these solids melt and react, releasing gases such as carbon monoxide and silicon monoxide, which flow rapidly up and out of the furnace. This, in effect, forms a counter-current flow within the furnace consisting of the descending solid raw materials and the rising hot gases. The heat and mass transfer processes both within and between the two phases depends strongly on exothermic chemical reactions that occur between the gas and the solid. However, despite control of these processes being vital to maintaining normal operating conditions in the furnace, they remain poorly understood.

In this talk, we develop a mathematical model for this counter-current flow, modelling the porous mix of raw materials as a solid perforated by a series of gas-filled channels. In a single channel, we model the gas as a multi-phase mixture, whose temperature is coupled to that of the surrounding solid by exothermic temperature-dependent chemical reactions occurring on the interface between the gas and solid phases. Utilising a combination of asymptotic and numerical methodologies, we investigate the temperature distribution and position of reactive regions predicted by the model, as both the type and rate of reaction, and channel geometry varies. Moreover, we identify parameter regimes that qualitatively match with behaviour observed in industrial furnaces and discuss what insights our model can provide to improve the operational management of furnaces. Keywords: Industrial mathematics; heat and mass transfer; compressible flow; reactive flow

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Nonlinear surface ring waves of moderate amplitude

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Loughborough University

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We study axisymmetric surface ring waves within the scope of 2D extended Boussinesq-type systems [1]. The extended cylindrical Korteweg - de Vries equation is derived to describe the far field evolution using asymptotic multiple scale expansions, and is similar to the model derived in [2] from the Euler equations. We then compare the performance of the reduced model with the full numerics developed for the original problem formulation, and identify the range of validity and limitations of the model.

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Constant work: Exploring feedback mechanisms in cellular mechanosensation

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Cells are active systems that respond to their environment. In particular, it is becoming increasingly apparent that physical force and the mechanical properties of their microenvironment play a crucial role in determining cell behaviour. Gaining a better appreciation of how these systems function may have significant implications for both tissue engineering applications and in understanding how mechanical factors affect the development and progression of a broad range of diseases such as cancer, osteoporosis, or cardiomyopathies. Here, we explore cellular contractility as a mechanism for mechanosensation. We take a theoretical continuum-mechanics approach, modelling cellular contractility as an active stress. The mathematical model is analysed and solved using both analytical approaches (exploiting approximations and symmetry arguments) and Finite Element Methods. We use this model to investigate energy constraints as a potential feedback mechanism, guiding how the cell may regulate its contractility in response to different environmental cues. We focus our model in the context of the most common biophysical experiments for mechanosensation where cells adhere to flat substrates with known mechanical properties. In such experiments the shape, size and pattern of adhesions between the cell and substrate, and distribution of contractility throughout the cell have significant implications for cellular mechanosensation. Hence, we also investigate the implications of these factors on cellular contractility, subject to our energy constraints. Keywords: mechanobiology, mechanotransduction, continuum mechanics, mathematical biology

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Phase-space formulation of the Full Lagrangian Approach for dispersed multiphase flows

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Dispersed multiphase flows occur in a variety of industrial and environmental contexts, with their omnipresence giving rise to the development of a range of modelling approaches for describing their behaviour. Of primary importance in the modelling of such flows is accurate representation of the spatial distribution of particles, which can exhibit wide variation in unsteady or turbulent flows. The full Lagrangian approach addresses this by tracking individual particles through the flow, and by computing the Eulerian-Lagrangian transformation tensor along trajectories as the flow evolves this method is able to provide the evolution of the local particle number density along each trajectory. Despite being an established method, the inherent drawback to this procedure is that singularities in the particle number density occur whenever trajectories cross in physical space, giving rise to unphysical contributions to the concentration field. This phenomenon occurs for inertial particles due to the multi-valued nature and nonzero compressibility of the particle velocity field, and the inherent dependence of trajectories on the particle velocity. To resolve this problem, it is necessary to consider particle motion within the full phase-space of particle variables which are tracked, specifically position and velocity. The uniqueness of trajectories in this phase-space is then guaranteed for a given set of initial conditions, with the implication that phase-space trajectories no longer intersect. Tracking the evolution of the phase-space probability density function (pdf) along trajectories therefore provides a well-defined methodology for avoiding the singularities which appear in number density where particle trajectories cross in position space, and results in a single-valued field representation for this pdf. In practice, reconstruction of the Eulerian pdf presents an issue in terms of computational tractability due to the high-dimensionality of the phase-space, however this can be mitigated by using an appropriate interpolation procedure. Specifically, it is demonstrated that using radial basis function interpolation with a judicious choice of kernel enables the Eulerian number density field to be directly computed from the Lagrangian phase-space pdf contributions. Results from a synthetic turbulent flow field are contrasted with both the conventional full Lagrangian approach and direct trajectory methods in order to exemplify the accuracy and computational efficiency of the proposed framework. Keywords: Continuum mechanics, Jacobian, Full Lagrangian approach, phase-space, particle-laden flows

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Effects of modelling assumptions on the arising dynamics in a cellular automaton model of tumour-immune interactions

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Prof. Helen Byrne, WCMB, University of Oxford; Prof. Philip Maini, WCMB, University of Oxford

Agent-based models allow the simulation of complex biological systems with detailed spatial resolution, and generate rich spatio-temporal datasets. In order to fully leverage the information contained within these simulated datasets, spatial statistics provide methods of analysis and insight into the biological system modelled, by quantifying inherent spatial heterogeneity within the system. Cellular automata are commonly used to model tumour-immune dynamics, due to their relatively simple and efficient design. Although the models are simple in design, many assumptions are made when constructing such models. We present a cellular automaton model of tumour-immune interactions and an analysis of the model dynamics, considering both the temporal and spatial evolution of the system. We use the model to investigate some of the standard assumptions made in these models, for example cell size and neighbourhood interactions, to assess the suitability of the models to accurately describe tumour-immune dynamics. Keywords: cellular automaton model; tumour-immune dynamics; spatial analysis

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Lateral Strain and Stress Concentration in Liquid Foam Fracture

Peter Stewart

University of Glasgow

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A monolayer of aqueous foam exhibits a brittle fracture mode under a rapidly applied driving pressure; this fracture propagates by cleavage of successive liquid films, driven by interfacial instability, and qualitatively resembles brittle fracture in solids. A discrete model, which incorporates the underlying film instability as well as viscous resistance from the moving liquid structures, predicts steady brittle fracture for large driving pressures. In line with experiments, this model predicts a range of inaccessible steady fracture velocities for driving pressure below a critical threshold. We show that this 'velocity gap' is also predicted by a one-dimensional continuum model, from which we can explore the limits of large film dissipation and large Plateau border dissipation. However, two-dimensional discrete simulations show a systematic dependence of propagation speed and critical fracture stress on the width of the foam channel (its dimension perpendicular to the direction of fracture), indicating the importance of dynamical processes in the lateral direction. Here we extend the continuum theory to two spatial dimensions, uncovering a peculiar, width-dependent mechanism of lateral strain concentration. The resulting fracture

dynamics and anisotropic stress fields are compared and contrasted with experiments, discrete simulations, and classical continuum fracture mechanics. Keywords: fracture mechanics; solid mechanics; gas-liquid foams; material science;

Scattering of an Ostrovsky Wave Packet in a Delaminated Waveguide

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Nottingham Trent University

Doctor Matt Tranter, Nottingham Trent University

In this talk I will discuss the scattering of an Ostrovsky wave packet, generated from a solitary wave, in a two layered waveguide with a delamination in the centre and soft (imperfect) bonding either side of the centre. The lower layer of the waveguide is assumed to be significantly denser than the upper layer, leading to a system of Boussinesq-Klein-Gordon (BKG) equations. Direct numerical modelling is difficult and so I will use a semi-analytical approach consisting of several matched asymptotic multiple-scale expansions, which leads to Ostrovsky equations in soft bonded regions and Korteweg-de Vries equations in the delaminated region. The semi-analytical approach and direct numerical simulations are in good agreement. I will also discuss how the dispersion relation is used to determine the wave speed and hence classify the length of the delamination, in addition to changes in the amplitude of the wave packet. These results can provide a tool to control the integrity of layered structures.
Keywords: Ostrovsky wave, delamination, Boussinesq-Klein Gordan equations

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An Ultra-weak Discontinuous Galerkin method for Two-Dimensional Elliptic Problems

Helmi Temimi

Gulf University for Science & Technology

In this work, we present and analyze a new ultra-weak discontinuous Galerkin (UWDG) finite element method for the following two-dimensional classical Poisson's equation subjected to the mixed Dirichlet-Neumann boundary conditions. Without loss of generality, in our analysis, we assume that all boundary condition functions are given smooth on their domains. The UWDG finite element approximations is used in the two space variables. The new UWDG discretization is presented in detail, including the definition of the numerical fluxes, which are necessary to obtain optimal error estimates. The proposed scheme can be made arbitrarily high-order accurate in two-dimensional space. The error estimates of the presented semi-discrete and fully-discrete schemes are both analyzed. Several numerical examples are provided to confirm the theoretical results.
Keywords: Ultra-weak discontinuous Galerkin method; elliptic problems; method of lines; convergence; a priori error estimation

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Matrix Wiener-Hopf equations and the implicit quadrature scheme

Ian Thompson

University of Liverpool

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Physical problems that involve an abrupt change in boundary conditions (e.g. due to a sharp edge) can often be reduced to Wiener–Hopf equations. Scalar Wiener–Hopf equations can be solved using a standard procedure [1], but no general method for solving coupled, or matrix, Wiener–Hopf equations has been discovered. A narrow class of matrix equations can be solved using a procedure due to Khrapkov [2,3], but many equations cannot be reduced to the necessary form. Approximating solutions to Wiener–Hopf equations is difficult because there is a delicate coupling between the behaviour of the unknown functions in the complex plane and at infinity. Local approximations that work in a restricted domain are likely to have the wrong singularity structure elsewhere, and often lead to physically implausible solutions.

In this presentation, we will discuss the 'implicit quadrature scheme,' a procedure for reducing Wiener–Hopf equations to linear systems of algebraic equations. This method does not rely on obtaining an approximate equation that can be expressed in Khrapkov form, but instead solves the Wiener–Hopf equation directly, in a single step. The implicit quadrature scheme was originally introduced in [4], for a problem in which the unknown functions are analytic at infinity. Here we will discuss the application of the method to matrix Wiener–Hopf equations in which the unknown functions have branch points at infinity.

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Keywords: Waves, complex analysis, Wiener-Hopf technique

Reconfigurable capillary self-assembly

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Inspired by recent experiments involving overdamped, microscopic colloids, we herein study experimentally and theoretically the structural rearrangements between ground states of clusters of millimetric spheres bound by capillary attractions. The structural rearrangements are driven by chaotic Faraday waves, which in turn play the role of an active bath. In contrast to colloids, inertial effects are non-negligible in our macroscopic system, prompting the development of a Langevin model of the particle dynamics, informed by the fundamental aspects of the fluid system. Our highly tunable experimental system addresses the relative paucity of model systems for studying inertial active and driven matter and informs new directions for non-invasive, reconfigurable self-assembly at the macroscale. Keywords: Experimental fluid mechanics; interfacial fluid mechanics; self-assembly; active and driven matter

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Laminar drag reduction in surfactant-contaminated superhydrophobic channels

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While superhydrophobic surfaces (SHSs) show promise for drag reduction applications, their performance can be compromised by traces of surfactants that accumulate at liquid-gas interfaces, generating Marangoni stresses that increase drag. This question is addressed for a three-dimensional laminar flow in a plane periodic channel with SHSs along both walls, in the presence of soluble surfactant. We consider the regime in which bulk diffusion is sufficiently strong for concentration gradients normal to the SHSs to be small. Seeking solutions that are periodic in the streamwise and spanwise directions, and exploiting a long-wave theory that accounts for rapid transverse Marangoni-driven flow and shear-dispersion effects, we derive a one-dimensional model for the distribution of interfacial and bulk surfactant. This exhibits multiple asymptotic regimes. Some are characterised by shear-dispersion and diffusion-dominated processes, where the liquid-gas interface exhibits shear-free behaviour and the drag reduction is at its maximum. In contrast, other regimes are dominated by Marangoni effects, where the liquid-gas interface exhibits no-slip behaviour and the drag reduction vanishes. Asymptotic solutions are constructed,

which compare favourably with the numerical solution to the model. The three-dimensional flow field is evaluated using Chebyshev collocation, domain decomposition and singularity removal techniques. This analysis provides a guide for designing surfactant-contaminated SHSs to maximise the drag reduction for applications and gives insight into regimes that are not included in current models, which assume constant shear at the interface. Keywords: Marangoni convection, drag reduction, microfluidics

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Emergent pseudo time-irreversibility in the classical many-body system of pair interacting particles

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One of the unsolved problems in physics is the origin of the thermodynamic arrow of time. In essence, while the solutions of governing equations of matter operating on microscopic scales are time-reversible, macroscopic-scale spatial order is known to solely decay in spontaneous processes. Since time-reversibility is not related to the number of degrees of freedom, it should not emerge on any scales in time-reversible mathematical models. This apparent contradiction is known as Loschmidt's paradox.

The problem was partly resolved by applying Poincare's recurrence theorem to prove the existence of pseudo time-irreversible solutions with practically infinitely large recurrence times. In addition, incorporating irreversibility in statistical physics based models led to the emergence of well-known phenomenological equations describing the macroscopic-scale diffusion of mass, momentum and energy. Unfortunately, since time-reversibility of the solution of the Liouville equation is directly broken in this framework by manually building in a stochastic component called the "Markovian assumption", the paradox cannot be fully resolved in this framework. In 1993, Olla, Vardhan and Yau showed that the time evolution of the closed classical many-body system of pair interacting particles is governed by (time-reversible) inviscid Euler equations in the exact hydrodynamic limit. Their result suggests that scale itself does not indicate the emergence of the second law of thermodynamics. Consequently, - assuming that the microscopic model is complete - pseudo time-irreversibility can only emerge from special microscopic initial conditions, which is a very popular view.

In this talk, we provide numerical evidence of emerging pseudo time-irreversibility due to random initial conditions in the closed many-body system of pair interacting classical particles. To study the macroscopic-scale behaviour of the system, first we derive exact continuum equations to the Hamiltonian many-body dynamics in a scaling limit. Contrary to traditional coarse-grained models, the thermal component of the microscopic momentum density is present in the solution of our continuum equations in the form of a pseudo random field. We will demonstrate that macroscopic-scale spatial order decays in temporal processes starting from initial conditions consisting of a deterministic macroscopic-scale and a stochastic microscopic-scale component. We will also show that heat and momentum relax in a non-diffusional way, which - in accordance with several other theoretical results - indicates the incompleteness of the classical microscopic model of matter. Possible reasons and resolutions of the problem will be discussed. Keywords: many-body dynamics, scaling limit, hydrodynamics, weak solutions, thermodynamics, random fields, irreversibility

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Singularity formation in inverted film flow and transition to dripping

Dmitri Tseluiko

Loughborough University

Mark G. Blyth, Te-Sheng Lin

The flow of a liquid film under an inclined flat plate is investigated with the aim to analyse transition to dripping as the plate inclination angle is varied. Travelling-pulse solutions are analysed for a linearised-curvature thin-film model as well as for a full-curvature thin-film mode that permits accurate capture of the surface deformation near the dripping transition. To corroborate the results of the thin-film computations and to extend the discussion beyond the range of validity the thin-film models, the inverted-film structures are also analysed using boundary-element computations for Stokes flow. Keywords: thin-film flow, Stokes flow, boundary-element computations

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Robust trajectory tracking by a multicopter platform with dynamic and information disturbance

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Bhargav Jha, Ujjwal Gupta, and Tal Shima (Technion - Israel Institute of Technology, Haifa, Israel)

The problem of robust trajectory tracking by a multicopter platform under the influence of aerodynamic drag is considered. The non-linear model consists of ten differential equations terms of its inertial position, velocity and orientation. The control inputs are the mass-normalized thrust and the body rates. The drag coefficients are known with uncertainty. Using differential flatness property of the non-linear model and Jacobian linearization, the model is written down as a ten-dimensional linear system for positional, velocity and orientation errors (measured states) and constant drag components (unknown states). The control inputs of the linearized system are the control discrepancies, whereas the dynamic disturbance is the vector of the body rates and the drag uncertainties. The state information is incomplete and noisy. The problem is formulated as a non-standard linear-quadratic differential game where the cost functional, along with the L^2-norm of the positional

and orientation error, includes quadratic penalty terms both for a dynamic and for an information disturbance. By the calculation of a program maximin, it is proved that this differential game is solvable subject to the non-singularity of some time-dependent matrix. The solvability condition is formulated in terms of the control, disturbance and noise penalty coefficients. The optimal control is constructed based on the solution of a Riccati matrix differential equation. Simulation results show a good tracking accuracy comparing with the previous approach not taking into account the drag uncertainty. Keywords: robust tracking; multicopter dynamics; linear-quadratic differential game; state uncertainty

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Vortex Leapfrogging external to a circular cylinder

Dr Matthew Turner
University of Surrey

In this talk we investigate the interaction of two line vortices of differing strengths in the presence of a circular cylinder. We will show that depending upon the initial positions of the vortices they will either undergo a periodic leapfrogging motion as they rotate around the cylinder, or they will move around the cylinder with no leapfrogging. We will derive an explicit criteria which separates these different behaviours of the system. Numerical results for initial vortex positions which do, and do not satisfy this criteria are presented to demonstrate the different motions available, as well as the robustness of the criteria. Keywords: vortex dynamics, inviscid fluids,

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Turing bifurcations in reaction-diffusion equations with n components in a bulk-surface system on a sphere

Edgardo Villar-Sepúlveda
University of Bristol
Alan Champneys - University of Bristol

It has been proven that many different real-world models show Turing instability patterns. These patterns have caught the interest of many people around the world since their existence reveals conditions under which some species can show oscillatory shapes throughout space. Up to now, much work has been done on Turing bifurcations on the line. Some insights have been developed on the conditions in which they can occur and their criticality. This concept provides an idea of the stability of the patterns that arise from a homogeneous steady state at the bifurcation point. However, not much has been said in different geometries. My talk will be about the formulation of general reaction-diffusion equations in a bulk-surface system with n components on a sphere, which can be thought of as a cell, for instance. I will show the conditions required by these systems to go through a Turing bifurcation and provide a way to know its criticality. Besides, I will show some figures to explain

the main ideas of my talk and some examples where I have applied my formulation. Keywords: Turing bifurcations, nonlinear dynamics, bulk-surface, reaction-diffusion equations

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The effects of rapid yawing on simple swimmer models and planar Jeffery's orbits

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UCL

Kenta Ishimoto (RIMS, Kyoto), Eamonn A. Gaffney (Oxford), Clément Moreau (RIMS, Kyoto), Mohit P. Dalwadi (UCL)

Over a sufficiently long period of time, or from an appropriate distance, the motion of many swimmers can appear smooth, with their trajectories appearing almost ballistic in nature and slowly varying in character. These long-time behaviours, however, often mask more complex dynamics, such as the side-to-side snakelike motion exhibited by spermatozoa as they swim, propelled by the frequent and periodic beating of their flagellum. Many models of motion neglect these effects in favour of smoother long-term behaviours, which are often of greater practical interest than the small-scale oscillatory motion. Whilst it may be tempting to ignore any yawing motion, simply assuming that any effects of rapid oscillations cancel out over a period, a precise quantification of the impacts of high-frequency yawing is lacking. In this talk, we will systematically evaluate the long-term effects of general high-frequency oscillations on translational and angular motion, cast in the context of microswimmers but applicable more generally. Via a multiple-scales asymptotic analysis, we will show that rapid oscillations can cause a long-term bias in the average direction of progression. We will identify sufficient conditions for an unbiased long-term effect of yawing, and will quantify how yawing modifies the speed of propulsion and the effective hydrodynamic shape when in shear flow. Furthermore, we will find and justify a surprising long-time validity of the derived leading-order solutions through a higher-order analysis, and summarise a rigorous justification of the applicability of our analysis to canonical microswimmers. Keywords: Asymptotic analysis; active particles; microswimming

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The three-dimensional sessile droplet on a non-flat substrate

Chung-Hao Wang
University of East Anglia
Alexander Korobkin

A droplet is placed on a solid surface, called the sessile drop. We investigate the three-dimensional static problem for droplet shape, in which the contact line is an unknown. The shape of the droplet is modelled using the Young-Laplace equation. For a flat substrate with an axisymmetric configuration, the solution for droplet shape is well known. However, if the droplet is placed on a non-flat substrate and the shape is non-axisymmetric, the problem is more complicated and requires a more sophisticated solution method. We introduce a stretched radial coordinate to simplify the mathematics, and non-dimensionalise the problem. The system is then solved asymptotically. We show that at leading-order, the axisymmetric problem is recovered, and we then present our findings for the first correction. Keywords: Sessile drop, Asymptotic analysis, Surface tension

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Minimal Reaction Systems Exhibiting Turing Instabilities

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Christian Yates (CMB & Dept. of Math. Sciences, University of Bath), Jonathan H. P. Dawes (CNCB & Dept. of Math. Sciences, University of Bath)

Turing instabilities in spatially continuous media are often studied through illustrative systems of differential equations for two (or more) scalar variables corresponding to the concentrations of interacting chemical species, for example the Schnakenberg or Brusselator models. These models contain polynomial nonlinear terms of cubic order which imply, at the level of individual chemical reactions, three molecules interacting simultaneously; trimolecular reactions. Such trimolecular reactions are however, improbable and therefore unphysical. Further, their high order can complicate spatial simulations of reaction-diffusion systems. Arguments that cubic terms might arise due to the rapid formation of intermediate complexes serve only to increase the conceptual complexity of the underlying chemical processes.

By focussing on simple PDE models of two species systems under the assumptions of mass-action kinetics and large particle numbers, we show that trimolecular reactions are in fact not necessary for a Turing instability to occur. Restricting to only reactions of at most second order, and by recasting the local linear stability and spatial instability conditions into requirements on reaction stoichiometries, we are able to establish necessary conditions for Turing instability. In turn, this allows us to deduce lower bounds on the necessary numbers of reactions of different orders that must be present.

In conclusion we are able to present a classification of 'minimal' Turing-unstable reaction schemes. Keywords: Turing instability; Turing pattern; chemical kinetics; PDE analysis; mathematical biology

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Relating the Milankovitch Cycles to Earth's Climate

Liam Wheen
The University of Bristol
Oscar Benjamin, Cameron Hall

For the last 3 million years, the Earth has exhibited glacial cycles, in which global ice volume oscillates in a near-periodic manner. The periodicity of the glacial cycles is closely correlated to those of the Milankovitch cycles, which describe variations in Earth's orbit. However, it is unclear how the solar energy changes associated with the Milankovitch cycles could produce the significant climatic changes observed through palaeothermometry.

In this talk, we present and explore a simple, physically-motivated differential equation model of climate, driven by the Earth's orbital parameters. Our model aims to isolate the Earth-based mechanisms that could provide the feedback required for the Milankovitch cycles to explain the significant variation in ice volume seen in data. As a result, our work creates a tool that could be used to explore hypotheses around the physical mechanisms underlying the past, and future, of the global climate.

Keywords: ice ages, Milankovitch cycles, nonlinear dynamics

Sound Propagation in Slowly Varying, Lined, Ducts

Tom White
The University of Manchester
Raphael Assier, William Parnell, The University of Manchester

Noise pollution is not only an annoyance, but can lead to serious health issues, with the WHO reporting that 18,000 premature deaths come as a result of traffic (road and air) induced cardiovascular disease. Therefore, it is important to have accurate models for sound propagation in systems such jet engines in order to control noise pollution.

Sound can be absorbed by lining ducts with locally reacting acoustic liners, which can be modelled by a frequency-dependent impedance boundary condition. Sound propagation in straight ducts is now well understood thanks to the study of the so-called modal solutions. Modal solutions are a useful modelling tool as they provide insight into the effectiveness of a specific liner impedance independent of forcing terms and allow for easier optimisation of liner properties.

In practise, the systems considered are not perfect cylinders and we must therefore consider the case of ducts with slowly-varying boundaries. With the aim of preserving the modal solutions analysis approach, the WKB (Wentzel-Kramers-Brillouin) approximation is used. The approximation assumes that in a slowly varying domain, modal solutions do not change eigenstate and there is no excitation/reflection of additional modes along the duct.

By considering a small parameter ϵ, relating the rate of change of the duct boundary, we can follow the analysis of Rienstra (1999) to find the behaviour of acoustic modes which vary slowly along the length of a duct. In this talk we will

look at a possible extension of Rienstra's seminal work to higher order in ϵ. The semi-analytic solutions are compared with numerical solutions to validate the method.
Keywords: acoustics, aeroacoustics, aymptotic analysis, waves

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Rivulet flow over and through a porous membrane

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Abdulwahed S. Alshaikhi and Brian R. Duffy (both University of Strathclyde)

Motivated by small-scale natural and industrial processes involving flow over and/or through a layer of a porous medium, a mathematical model for the steady gravity-driven flow of a rivulet of fluid with finite width over and through a permeable membrane is formulated and analysed. The three-dimensional shape of the free surface of a rivulet with either fixed semi-width or fixed contact angle is determined, and it is shown how the length, base area and volume of the rivulet on the permeable part of the membrane depend on the physical properties of the system. In particular, whereas there is a physically realisable pendant rivulet solution only if the semi-width does not exceed a critical value, there are physically realisable sessile and vertical rivulet solutions for all values of the semi-width; moreover, a sessile rivulet with fixed semi-width has a finite maximum possible length which is attained in the limit of a wide rivulet. Further details are given in Alshaikhi, Wilson and Duffy [Phys. Rev. Fluids 6, 104003, (2021)]. Keywords: rivulet, porous membrane, thin-film flow

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Influence of glacier algae on ice sheet surface melt

Tilly Woods
University of Oxford
Ian Hewitt (University of Oxford)

The runoff from the Greenland ice sheet is a significant contribution to sea level rise. During the past few decades, the Greenland ice sheet has been darkening in colour, leading to a lowering of the surface albedo, hence an increase in surface melting and runoff. This darkening is in part due to the presence of dark-coloured 'glacier algae' on the bare ice surface of the ablation zone. The glacier algae exist in the thin surface layer of partially saturated porous ice known as the 'weathering crust'. It has been proposed that there is a potential positive feedback loop between algae, albedo, melting and weathering crust evolution, but this feedback is yet to be studied mathematically.

Here, we construct a one-dimensional continuum model to describe the near-surface flow of meltwater through porous ice, the structure of which is evolving due to melting and refreezing. We include a two-stream approximation of penetrating solar radiation in our model to capture the formation of the weathering crust. To this weathering crust model, we couple a simple logistic-growth-based model for the

evolution of glacier algae and their nutrients, in order to investigate the potential feedback loop. We consider steady state solutions of our model both with and without the dependence of albedo on algae to determine how the presence of glacier algae impacts surface melting and runoff. Keywords: Geoscience; continuum modelling; phase change; porous media; mathematical ecology

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Stochastic synchronisation in non-locally coupled, noisy oscillators

Jeremy Worsfold
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Synchronisation of non-locally coupled oscillators has been extensively studied since Kuramoto's model of oscillators was proposed in 1975 [1]. This model has been extended to oscillators with intrinsic, independent noise for which partial synchronisation can still occur [2]. All of these models focus on the continuum limit when realistic systems are usually finite. In this talk, we explore how stochastic synchronisation can occur for finite populations. This is formulated as a McKean-Vlasov type model for interacting Brownian particles. From this we describe the fluctuations due to the finite sized effects.

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[2] Juan A. Acebrn, L. L. Bonilla, Conrad J. Pérez Vicente, Félix Ritort, and Renato Spigler Rev. Mod. Phys. 77, 137 - Published 7 April 2005 Keywords: Dynamical systems, Synchronisation, Collective behaviour, Interacting particle systems

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Magneto-thermoelastic interactions in a nanostructured micropolar orthotropic solid half-space with impedance boundary

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In this article, the governing partial differential equations for nonlocal micropolar orthotropic magneto-thermoelastic half space with impedance boundary in context of generalized theory of thermo-elasticity for x-z plane are obtained. The plane wave solutions of these equations indicate the existence of four coupled quasi plane waves in the plane namely quasi-longitudinal displacement (qCLD) wave, quasi transverse displacement (qCTD) wave, quasi transverse microrotational (qCTM) wave and quasi thermal wave (qCT). Reflection of these plane waves from the surface having impedance boundary is studied to obtain the expression for reflection coefficients and energy ratio of various reflected waves. Reflection coefficients and energy ratios of various reflected waves are computed numerically for a particular material and the effects of magnetic field, nonlocal, impedance parameters and angle of incidence are shown graphically on these reflection coefficients and energy ratios. Keywords: wave propagation, anisotropy, reflection

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Mathematical and in vitro modelling of high shear thrombosis in a long, thin, microfluidic system

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Thrombosis under pathologically high shear stresses relies on the protein Von Willebrand Factor (VWF). At high shear rates VWF unfolds, which exposes binding sites, and facilitates rapid platelet deposition and clot formation. Accurate prediction of clotting dynamics under high shear is a key part of developing safe and effective treatments. We develop a reduced mathematical model for the initial stages of thrombosis and validate the model using in vitro data.

We examine thrombosis in a rectangular, venturi-style microfluidic system. We exploit the small aspect ratio of the microfluidic system to construct a reduced continuum model. The model includes a novel mechanistic description of VWF dynamics using a dilute limit of a viscoelastic fluid model. We parameterise the mathematical model using in vitro data of platelet deposition over time in the microfluidic system. The validated model is used to investigate the effect of varying stenosis geometry and blood flow conditions on the unfolding of VWF and subsequent platelet binding.

Keywords: fluid mechanics, asymptotic analysis, physiological flows

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Blow-up analysis of fast-slow PDEs with fold type singularities

Thomas Zacharis

University of Edinburgh

Nikola Popovic - University of Edinburgh, Mariya Ptashnyk - Heriot-Watt University, Christian Kuehn - Technical University of Munich, Maximilian Engel - FU Berlin, Felix Hummel

We study a fast-slow, reaction-diffusion PDE system, consisting of two equations on a bounded domain, with a fold singularity in the reaction term of the fast variable, while the slow variable assumes the role of a dynamic bifurcation parameter. This extends the classical fast-slow dynamic fold bifurcation problem to an infinite-dimensional setting. Our approach is to use a spectral Galerkin discretization and use the techniques of Geometric Singular Perturbation Theory (GSPT) on the resulting high-dimensional ordinary differential equation systems. In particular, away from the fold singularity we obtain the existence of invariant manifolds, while in a neighbourhood of the singularity we using geometric desingularization via a blow-up method. A key ingredient is the inclusion of the domain length of the PDEs as a variable. Finally, we connect the invariant manifolds obtained through this discretization process with invariant manifolds that exists in the original phase space of the PDE system. Keywords: dynamical systems; PDE dynamics; geometric desingularization; singular perturbations; invariant manifolds

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Identification of individual traits in collective behaviour of animal groups

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In the recent literature, much attention has been paid to the impact of individual characteristics on collective outcomes. While advances in computer vision tools have made it easier to observe, for example, collective motion, it is still challenging to identify the relevant traits of a large number of individuals. Future progress in this area could benefit immensely from developing tools that allow traits to be inferred from data that can typically be recorded at the group level. Here we propose to use the diffusion map, a convenient manifold learning technique, to infer traits from recordings of collective motion. We simulate the motion of a school of fish which heterogeneous movement traits. This simulation provides a ground truth where we know the underlying traits and the resulting trajectories. We then ask if the individual traits can be inferred from trajectory information, i.e. data that could have been captured in an actual experiment. Our results show that the diffusion map is able to identify relevant traits with good accuracy. Importantly, trait estimation is almost parameter-free and does not depend on conjectures regarding the nature of the relevant trait variables. Based on these results, it is reasonable to believe that a similar approach could be used to identify individual traits and potentially discover new trait axes directly from lab recordings available recording of animal groups. Keywords: collective dynamics, diffusion map, nonlinear manifold learning, agent-based modelling, network science, data-driven methodology

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Dynamics of particle aggregation in evaporating and de-wetting films of complex liquids

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Department of Mathematical Sciences, Loughborough University

David N. Sibley, Dmitri Tseluiko, Andrew J. Archer

We consider dynamic wetting and de-wetting processes of complex liquid droplets focusing on the case of colloidal suspensions, where the particle interactions cause agglomeration. This leads to interesting dynamics of the droplet surface. Incorporating concepts from thermodynamics, we construct a model consisting of a pair of coupled partial differential equations that represent the evolution of the droplet and the effective colloidal height profiles using the thin-film approximation. The model extends also to include mass transfer effects by allowing the solvent to evaporate. We determine the relevant phase behaviour of the uniform system, including finding associated binodal and spinodal curves helping to uncover how the emerging behaviour depends on the particle interactions. Performing a linear stability analysis of our system enables us to identify parameter regimes where agglomerates form, which we independently confirm through numerical simulation. We obtain various dynamics such as uniform colloidal profiles in an unstable situation evolving into agglomerates and thus elucidate the interplay between evaporation, de-wetting and particle aggregation in complex liquids on surfaces. We predict the phase separation behaviour of colloids according to the dispersion relations and achieve agreement between the theoretical predictions and computational results. Keywords: Droplets, Interfacial flows, Multiphase flows, Thin-film flows

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Free Surface Waves for a Lamb-Oseen Vortex Flow

Emanuele Zuccoli

University of Warwick

E. J. Brambley (University of Warwick) - D. Barkley (University of Warwick)

The response to small perturbations to a free surface Lamb-Oseen vortex flow in a laterally unbounded domain has been investigated numerically. Despite various type of waves that can arise, those of major interested have been surface waves as they have been observed in experiments more easily. Surface waves lead the dynamics of the system for moderately high and high azimuthal wavenumber perturbations and their behaviour changes as the speed of the vortex increases, ultimately reaching a neutral stability state. In analogy to a quantum mechanical system, such states correspond to Quasi-bound States (QBs), i.e. normal modes whose decay rate in time is null and whose corresponding eigenfunctions remain trapped in a narrow region where the base flow is maximum. Quasi-bound States have been already shown to appear in shallow water surface waves due to small perturbations of a bathtub vortex. In our work we have shown that such states also exist for a purely rotating flow in a deep water regime. The mechanism underlying the change of character of surface waves can be found in the interaction between the waves and the base flow; as long as the velocity of the vortex is sufficiently small waves extract energy by the base flow and radiate it towards the exterior of the vortex core. On the contrary, as the rotation speed of the flow gets higher, waves remain trapped. Such a mechanism also has implications on the direction of propagation of the waves with respect to the vortex. Keywords: Free Surface Flows - Water Waves - Linear Stability Analysis - Vortex Flows

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Minisymposia abstracts

Multi-scale modelling of magnetic nanoparticles delivery and heat transport in vascularized tumour

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University of Glasgow

Raimondo Penta, and Radostin Simitev. University of Glasgow

Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

We derive a new system of homogenised partial differential equations (PDEs) describing blood transport, delivery of nanoparticles, and heat transport and apply it to investigate cancer hyperthermia driven by the application of the magnetic field applied to Iron oxide nanoparticles. The new model comprises a double Darcy's law, coupled with two double advection-diffusion-reaction system of PDEs describing fluid, particles and heat transport and mass, drug, and heat exchange. The role of the micro-structure is encoded in the coefficients of the model which are to be computed solving appropriate periodic problems. We study the influence of vessels geometry as the tumour vessels are not regular and their tortuosity varies within the tumour. In addition, we investigate temperature maps by using different injection conditions. The temperature should be above 42 to destroy cancer cells but for at most one hour to avoid heating the surrounding healthy tissue. We determine the best magnetic intensity, injection time, wall shear rate, and concentration of nanoparticles to achieve the above-mentioned condition.

On the role of elasticity in the quasi-static decohesion of biological systems

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Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

In this contribution, we consider a mathematical model addressing the mechanical interactions occurring in certain classes of biological structures and, as a reference example in this field, we focus our attention on focal adhesions (see, for instance, [1, 2] and references therein). Staring from [1, 2], we study the occurrence of decohesion

and its modulation provided by the elastic properties of the system in the passive regime. We propose a one-dimensional approach in which both the focal adhesion and the substratum to which it is anchored are modelled as linear elastic straight fibres. In addition, following [3, 4], we consider a variational scheme by taking inspiration from the Griffith's theory of fracture. This allows us to determine local and global minima of the total energy associated with the system under study, which accounts for two contributions: one is associated with the elastic properties of the system, the other one pertains to the detachment process. As a result, the proposed model is able of capturing some macroscopic mechanical quantities of the system and the advancement of the decohesion front. In particular, the model resolves the transition from a ductile to fragile regime of rupture. Interestingly, our predictions fulfil a qualitative and quantitative agreement with well-known results regarding the saturation of the limit decohesion force in biological systems [5, 6].

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Influence of remodelling in a biphasic multicellular aggregate: stress-relaxation and shape recovery

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Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

Multicellular aggregates are considered a good case of study for understanding other, more involved, biomechanical problems. For example, within the context of the research on cancer [1], the early stages of the formation of tumours are heavily influenced by mechanical aspects.

In particular, we take inspiration from [2], in which a three-dimensional, elasto-plastic, mono- phasic (solid) model is developed. Hence, we describe the multicellular aggregate as a saturated

biphasic medium comprising a porous matrix, whose remodelling of its internal structure is described in terms of an isochoric plastic-like process, and an interstitial fluid, for which we assume Darcian regime. We specialise the model to a compression-release test, in which a prescribed displacement is applied through the movements of the two plates between which the aggregate is inserted [2,3]. The results of our numerical simulations permit to evaluate, with respect to experimental data [4], the elastic response of the aggregate, in particular in the form of stress relaxation curves and shape recovery curves. We conclude focusing on the consequences of the coupling between the fluid and remodelling.

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Multiphase Flow in Dual Scale Porous Media during Resin Infusion Process of Composite Manufacturing

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Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

Resin infusion is a pressure-gradient-driven composite manufacturing process in which the liquid resin is driven to flow through and fill in the dual scale void space of a porous composite preform prior to the heat treatment for resin solidification. It usually is a great challenge to design both the infusion system and the infusion process meeting the manufacturing requirements, especially for large-scale components of aircraft and wind turbine blades. The major issues during manufacturing are: 1) structural scale dry domains where resin flow cannot reach, 2) material scale air bubbles trapped in inter- or intra-fibre-bundles void space, 3) resin rich domains where the volumetric fraction of fibre is so low that fibres do not play its role of reinforcement as designed. All of those issues happening during the manufacturing process may lead to incomplete products or defects which become the sources of fracture.

Aiming at addressing the key concerns about flow fronts and air bubble entrapment, the present study proposes a modelling framework of the multiphase flow of resin and air in a dual scale porous medium, i.e. a composite preform. A finite strain formulation is discussed for the fluid-solid interaction during an infusion process. The present study bridges the gap between the microscopic observation and the macroscopic modelling by using the averaging method and first principle method, which sheds new light on the high-fidelity finite element modelling.

Finite element simulation is also presented to demonstrate the process of resin infusion.

Double poroelasticity derived from the microstructure

Laura Miller
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Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

We derive the balance equations for a double poroelastic material which comprises a matrix with embedded subphases. We assume that the distance between the subphases (the local scale) is much smaller than the size of the domain (the global scale). We assume that at the local scale that the matrix and the subphases can be described by either Biot's anisotropic, heterogeneous, compressible poroelasticity (i.e., the porescale is already smoothed out), or for particular applications, as a poroelastic composite. We then decouple the spatial variations by means of the two-scale homogenization method to upscale the interaction between the poroelastic phases at the local scale. This way, we derive the novel global scale model which is formally of poroelastic-type. The global scale coefficients account for the complexity of the given microstructure and heterogeneities. These effective poroelastic moduli are to be computed by solving appropriate differential periodic cell problems. The model coefficients possess properties that, once proved, allow us to determine that the model is both formally and substantially of poroelastic-type. The properties we prove are a) the existence of a tensor which plays the role of the classical Biot's tensor of coefficients via a suitable analytical identity and b) the global Biot's modulus is positive. We can obtain a solution to the novel model encoding structural detail on three scales. The problems found in this work contain coefficients that are determined by solving the cell problems from the finer hierarchical level. These finer scale cell problems are the standard cell problems of poroelasticity and the cell problems for a poroelastic composite. This approach can be applicable to many biological scenarios including cardiac myocytes within the myocardium.

A Quasilinear Viscoelastic Model for the cyclic compression of all-polymer syntactic foams

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Zeshan Yousaf, William J. Parnell (University of Manchester); Riccardo De Pascalis (Universit'a del Salento)

Minisymposium: Advances and challenges in the modelling of multiscale, complex, and heterogeneous materials

In the present study, a quasi-linear viscoelastic (QLV) (compressible) continuum model was developed to determine the time-dependent constitutive properties of all-polymer syntactic foams with various filling fractions under cyclic compression. These syntactic foams were produced by inserting hollow polymer microspheres with polydisperse diameters (in the range of 10-100 microns) and wall thicknesses (in the

range 150-250 nm) into a polyurethane matrix. Firstly, the loading and unloading tests were performed to large strain, illustrating the compressibility, recoverability and energy dissipation properties of the foams. Then a range of strain energy functions (SEF) were employed (e.g. Neo-Hookean, Horgan-Murphy and Ogden), in the modification of Fung's QLV model described in [1]. By optimizing the fit to the model, the physical properties of the foams are deduced over a range of strains and volume fractions of fillers. Coefficients in the SEFs are also found. As well as being of key industrial interest in a variety of syntactic foam applications, such models, and associated optimization techniques linked to experimental data, are of significant utility in a range of other scenarios, e.g. in the case of soft tissues, for example.

Structural and practical identifiability of ERK kinetics

Emilie Dufresne
University of York
Lewis Marsh, Helen Byrne and Heather Harrington, all at Oxford University.

Minisymposium: Applied Algebra and Geometry

This talk is based on a paper written in collaboration with Lewis Marsh, Helen Byrne and Heather Harrington, where we explored the algebra, geometry and topology of ERK kinetics. The MEK/ERK signalling pathway is involved in cell division, cell specialisation, sur- vival and cell death. We studied a polynomial dynamical system describing the dynamics of MEK/ERK proposed by Yeung et al. with their experimental setup, data and known biological information. The experimental dataset is a time-course of ERK measurements in different phosphorylation states following activation of either wild-type MEK or MEK mutations associated with cancer or developmental defects. My focus in this talk will be on identifiability, both structural and practical. Structurally identifiable is concerned with asking whether parameter values can be recovered from perfect data. Practical identifiability addresses the more realistic situation where we assume there is measurement noise. We observe that the original model is structurally but not practically identifiable. We will discuss how algebraic quasi-steady state approximation leads to a smaller simpler model which is both structurally and practically identifiable, while providing a probable explanation for the practical non-identifiability of the original model.

Linear programming complementation

Maximilien Gadouleau
Durham University
George B. Mertzios, Durham University and Viktor Zamaraev, University of Liverpool

Minisymposium: Applied Algebra and Geometry

In this talk, we introduce a new kind of duality for Linear Programming (LP), that we call LP complementation. We prove that the optimal values of an LP and of its complement are complement pairs (provided that either the original LP or its complement has an optimal value greater than one). The main consequence of the LP complementation theorem is for hypergraphs. We introduce the complement of a hypergraph and we show that the fractional packing numbers of a hypergraph and of its complement are complement pairs; similar results hold for fractional matching, covering and transversal numbers. This hypergraph complementation theorem has several consequences for fractional graph theory. In particular, we relate the fractional dominating number of a graph to the fractional total dominating number of its complement.

Representations of partial leaf sets in phylogenetic tree space

Gillian Grindstaff
Oxford University
Megan Owen, Lehman College, CUNY

Minisymposium: Applied Algebra and Geometry

The metric space of phylogenetic trees defined by Billera, Holmes, and Vogtmann, which we refer to as BHV space, provides a natural geometric setting for describing collections of trees on the same set of taxa. However, it is sometimes necessary to analyze collections of trees on non-identical taxa sets (i.e., with different numbers of leaves), and in this context it is not evident how to apply BHV space. Ren et al. approached this problem by describing a combinatorial algorithm extending tree topologies to regions in higher dimensional tree spaces, so that one can quickly compute which topologies contain a given tree as partial data. In this work, we refined and adapted their algorithm to work for metric trees to give a full characterization of the linear subspace of extensions of a subtree. We demonstrate how to apply our algorithm to define and search a space of possible supertrees and, for a collection of tree fragments with different leaf sets, to quantify their compatibility.

Algebraic Degree of Polynomially Constrained Optimization

Olga Kuznetsova

Aalto University

Muhammad Ardiyansyah, Aalto University; Kaie Kubjas, Aalto University; Luca Sodomaco, Aalto University

Minisymposium: Applied Algebra and Geometry

Consider an optimisation problem whose objective function is in the algebraic closure of the rational function field and the feasible set is an algebraic variety. The algebraic degree of a variety in a given optimisation problem is the number of complex critical points. Using radical parametrisation, we show that the notion of algebraic degree is well-defined for a certain large class of such problems. As a special case, we study the case of the p-th power of the p-norm, for which we generalise the notion of the ED correspondence variety and give explicit formulas for the algebraic degree.

Exact reductions of dynamical systems

Gleb Pogudin

LIX, CNRS, cole Polytechnique, Institute Polytechnique de Paris

Antonio Jimnez-Pastor (cole Polytechnique), Alexey Ovchinnikov (CUNY), Isabel Prez Verona (IMT Lucca), Mirco Tribastone (IMT Lucca), Xingjian Zhang (cole Polytechnique)

Minisymposium: Applied Algebra and Geometry

Dynamical systems are frequently used for modeling in the sciences. Building a detailed model often requires taking into account a large number of factors and, as a result, a model may become quite large. High-dimensional models with dozens or hundreds of state variables are not only challenging computationally but it is also hard to use them to derive mechanistic insights. Exact model reduction is a way to address this issue by finding a self-consistent lower-dimensional projection of the corresponding dynamical system. I will describe recent algorithms for computing such reductions (in particular the CLUE software https://github.com/pogudingleb/CLUE) and demonstrate them on the models from literature.

Active control of thin liquid film flows using a hierarchy of models

Susana Gomes

University of Warwick

Radu Cimpeanu (Warwick), Demetrios Papageorgiou (Imperial College London)

Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

The flow of a thin film down an inclined plane is a canonical setup in fluid mechanics and associated technologies, with applications such as coating, where the liquid-gas interface should ideally be flat, and heat or mass transfer, where an increase of interfacial area is desirable. In each of these applications, we would like to robustly and efficiently manipulate the flow in order to drive the dynamics to a desired interfacial shape. In this talk, I will propose a feedback control methodology based on same fluid blowing and suction through the wall. The controls will be developed in the lower (simpler) levels of a hierarchy of models for a falling liquid film based on reduced-order modelling and asymptotic analysis. The goal is to develop control strategies at these more cost-effective levels of the hierarchy and investigate their ability to translate across the hierarchy into real-life solutions by using direct numerical simulations of the Navier-Stokes equations, which in this context act as an in silico experimental framework. I will discuss distributed controls as well as (more realistic) point-actuated controls, their robustness to parameter uncertainties and validity across the hierarchy of models.

Stretches and Wobbles: Probing the stability and bifurcation of a dynamic contact line

Jack Keeler

University of Warwick

Satish Kumar, University of Minnesota; Duncan Lockerby, University of Warwick; James Sprittles, University of Warwick.

Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

The moving-contact line between a fluid, liquid and a solid is a ubiquitous phenomenon, and determining the maximum speed at which a liquid can wet/dewet a solid is a practically important problem. Using continuum models the maximum speed of wetting/dewetting can be found by calculating steady solutions of the governing equations and locating the critical capillary number, Ca_{crit}, above which no steady-state solution can be found. Below Ca_{crit}, both stable and unstable steady-state solutions exist and if some appropriate measure of these solutions is plotted against Ca, a fold bifurcation appears where the stable and unstable branches meet. In this talk we develop a computational framework to describe this phenomenon and, by applying ideas from dynamical systems theory to the highly-dimensional complex system, show that, rather than just being a consequence of the fold bifurcation, the unstable solutions have profound importance on the transient behaviour of the system. Significantly, the system can become unstable when $Ca < Ca_{\text{crit}}$ due to finite amplitude interfacial 'wobbles' are more dangerous than 'stretch' perturbations.

Exploring a new dimension in high-speed liquid-liquid impact

Matthew Moore
University of Hull
Radu Cimpeanu (University of Warwick)

Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

Droplet-liquid impacts are fundamental to a range of industrial applications including spray cooling, fuel injection, pesticide spray distribution in the context of high precision agriculture and manufacturing applications such as inkjet printing and droplet-based 3D printing. The bulk of prior work on liquid impact problems focuses on axisymmetric, normal impacts due to the relative simplicity of experimental characterisation and visualisation, as well as reduced computational demands. In practice, however, non-axisymmetric impacts are far more common. Given the complexities, it is of paramount interest to exploit the interplay between analytical and numerical approaches with a view to gaining comprehensive insight into a challenging modelling scenario in which each technique in isolation would be either inefficient or completely unviable.

Building on the success of past comparisons in two-dimensional settings [1], we generalise the early time asymptotic theory of liquid-liquid impact to three dimensions and investigate its predictive capabilities, as well as its range of validity. We use the open-source Basilisk package as the backbone of our implementation, taking advantage of its parallelisation features (alongside considerable computational resources) in order to unlock previously inaccessible general impact scenarios. We focus on the characterisation of meaningful morphological features such as the location of the root of the ejected sheet, the shape of the latter, as well as velocities therein. The later stages of the impact (including formation of secondary droplets) are then interrogated numerically over a range of impingement angles. We also outline further modelling avenues in order to improve the proposed methodology [2].

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Lubrication layer driven capillary-scale rebound dynamics: A pesudo-spectral approach

Katie Phillips

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Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

A droplet about to impact a free surface must first make its way through a layer of air acting as a barrier preventing coalescence. In a millimetric regime, the capillary action of the free surface may dominate the dynamics of the interaction and is able to provide an upward kick to rebound the droplet prior the full evacuation of the air layer, which would have allowed coalescence. In such a regime, the trapped air acts as a lubrication layer between the impactor and the free surface. To leading order, such a millimetric droplet acts as a rigid sphere, allowing developments of numerical models for solid-liquid impacts to be a reasonable approximation of droplet dynamics. In this talk, we present the development of a 2D model of a millimetric solid sphere impacting on a free surface. We take a multi-scale approach to include the air layer as a dynamical component in the system by coupling an asymptotic derivation of the leading order problem, with psuedo-spectral methods to model the behaviour of the free surface, and smaller scale lubrication regime for the dynamics of the cushioning layer.

Sedimentation of Thin, Rigid Discs: An Augmented Finite-Element Method

Christian Vaquero-Stainer

University of Manchester

Matthias Heil and Draga Pihler Puzovic

Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

We present a numerical investigation of the behaviour of 2D, deformed circular disks sedimenting under gravity in a quiescent 3D viscous fluid at low Reynolds number. The sharp edge of such an object creates a singularity in the fluid pressure and the velocity gradient. At low Reynolds number, this means a significant contribution of the total drag comes from the vicinty of the disk edge; for a flat disk at zero Reynolds number, 30% of the total drag is generated by the outermost 5% of the disk radius. This implies that any under-resolution of the pressure and the velocity gradient leads to critical errors in the sedimentation velocity and rotation, but such singularities have a severe impact on the convergence rate of standard finite-element (FE) discretisations. To address this, we have developed a novel augmented FE method which allows analytic (singular) functions of unknown amplitude to be subtracted from the full solution in a sub-domain around the disk edge , rendering the FE remainder part of the solution regular and thus restoring the standard

FE convergence rate. The singular amplitudes are determined via PDE-constrained minimisation of a suitably chosen functional which captures the key signatures of the singularity.

Optimal control of multiphase flows

Alexander Wray
University of Strathclyde
Susana Gomes, Radu Cimpeanu (University of Warwick)

Minisymposium: At the interface between analytical methods and high performance computing in fluid mechanics

Multiphase flows are ubiquitous in nature and industry, and controlling them has applications everywhere from carbon sequestration to medical diagnostics. As a consequence, control has seen an ever-increasing focus in the field of fluid dynamics. Unfortunately, inverse problems of this type are typically extremely computationally costly, and most existing studies have focussed on single phase flows which admit convenient bases on which to project suitable reduced dimensional models. Multiphase studies have typically confined their focus to lubrication-type equations, which have limited applicability.

Here the more complex problem of free-surface flow down an inclined plane is examined, simulated using the volume-of-fluid open-source solver Basilisk. Control is implemented via developing an extremely high-fidelity reduced order model using a projection method akin to the Method of Weighted Residuals, and using a Model Predictive Control loop to control the direct numerical simulation with judicious use of the model. Actuation is achieved via imposing a spatiotemporally-varying electric potential on an electrode parallel to the substrate.

The model is investigated in detail, demonstrating a high degree of accuracy even into the short-wave regime. The control mechanism is shown to be applicable to both uniform and non-uniform target states, and the efficacy of the model predictive control loop is investigated across a wide variety of parameters.

Unified landslide hazard assessment using hurdle models

Daniela Castro-Camilo

University of Glasgow

Ms Erin Bryce and Dr Luigi Lombardo

Minisymposium: Decision making under uncertainty

Climatically-induced natural hazards are a threat to communities. They can cause life losses and heavy damage to infrastructure, and due to climate change, they have become increasingly frequent. This is especially the case in tropical regions, where major hurricanes have consistently appeared in recent history. Such events induce damage due to the high wind speed they carry, and the high intensity/duration of rainfall they discharge can further induce a chain of hydro-morphological hazards in the form of widespread debris slides/flows. The way the scientific community has developed preparatory steps to mitigate the potential damage of these hydro-morphological threats includes assessing where they are likely to manifest across a given landscape. This concept is referred to as susceptibility, and it is commonly achieved by implementing binary classifiers to estimate probabilities of landslide occurrences. However, predicting where landslides can occur may not be sufficient information, for it fails to convey how large landslides may be.

This work proposes using a flexible Bernoulli-log-Gaussian hurdle model to simultaneously model landslide occurrence and size per areal unit. Covariate and spatial information are introduced using a generalised additive modelling framework. To cope with the high spatial resolution of the data, our model uses a Markovian representation of the Matrn covariance function based on the stochastic partial differential equation (SPDE) approach. Assuming Gaussian priors, our model can be integrated into the class of latent Gaussian models, for which inference is conveniently performed based on the integrated nested Laplace approximation method. We use our modelling approach in Dominica, where Hurricane Maria (September 2017) induced thousands of shallow flow-like landslides passing over the island. Our results show that we can not only estimate where landslides may occur and how large they may be, but we can also combine this information in a unified landslide hazard model, which is the first of its kind.

Multilevel Double Loop Monte Carlo Method with Importance Sampling for Bayesian Optimal Experimental Design

Luis Espath

University of Nottingham

Joakim Beck (KAUST), Ben Mansour Dia (KFUPM), Raul Tempone (RWTH/KAUST)

Minisymposium: Decision making under uncertainty

An optimal experimental set-up maximizes the value of data for statistical inferences. The efficiency of strategies for finding optimal experimental set-ups is particularly important for experiments that are time-consuming or expensive to perform. When the experiments are modeled by Partial Differential Equations (PDEs), multilevel methods have been proven to reduce the computational complexity of their single-level counterparts when estimating expected values. For a setting where PDEs can model experiments, we propose a multilevel method for estimating the widespread criterion known as the Expected Information Gain (EIG) in Bayesian optimal experimental design. We propose a Multilevel Double Loop Monte Carlo (MLDLMC), where the Laplace approximation is used for importance sampling in the inner expectation. The method's efficiency is demonstrated by estimating EIG for inference of the fiber orientation in composite laminate materials from an electrical impedance tomography experiment.

Adaptive Multilevel Monte Carlo

Abdul-Lateef Haji-Ali

Heriot-Watt University

Jonathan Spence, Aretha Teckentrup

Minisymposium: Decision making under uncertainty

In this talk, I will discuss the challenges in computing probabilities of the form $P[X \in \Omega]$ where X is a random variable and Ω is a d-dimensional set. Computing such probabilities is important in many contexts, e.g., risk assessment and finance. A frequent challenge is encountered when only a costly approximation of the random variable X can be sampled. For example, when X depends on an inner expectation that has to be approximated with Monte Carlo or when X depends on a non-trivial (stochastic) differential equations and a numerical discretization must be employed. A naive Monte Carlo method has a prohibitive complexity that compounds the slow convergence of Monte Carlo with the complexity of approximation. On the other hand, a naive application of Multilevel Monte Carlo (MLMC) offers limited improvement to the computational complexity. After presenting these classical methods, I will discuss two strategies to improve MLMC when approximating the probability to the extent that its computational complexity becomes independent of the complexity of approximation.

Mutual Information for Explainable Deep Learning of Multiscale Systems

Eric Hall
University of Dundee
Sren Taverniers (Stanford University), Markos Katsoulakis (University of Massachusetts Amherst), Daniel Tartakovsky (Stanford University)

Minisymposium: Decision making under uncertainty

The timely completion of design cycles for complex engineered systems relies on rapid simulation-based prototyping. Such systems typically exhibit multiscale/-physics interactions and involve correlated/dependent control variables and non-Gaussian quantities of interest. We develop a model-agnostic, moment-independent global sensitivity analysis (GSA) that relies on differential mutual information to rank the effects of control variables on quantities of interest. Deep neural network surrogates can meet the data demands of GSA by replacing computationally intensive components of the underlying physics-based model. When viewed as an uncertainty quantification method for interrogating surrogates, the mutual information-based GSA assists in explaining surrogate predictions, thereby enabling surrogates to close design loops. Compatible with a wide variety of black-box models, we demonstrate that surrogate-driven mutual information GSA provides useful and distinguishable rankings for two applications of interest in energy storage. Consequently, our information-theoretic GSA provides an outer loop for accelerated product design by identifying the most and least sensitive input directions and performing subsequent optimization over appropriately reduced parameter subspaces.

Randomized multilevel Monte Carlo for inference

Kody Law
University of Manchester

Minisymposium: Decision making under uncertainty

Often in the context of data centric science and engineering applications, one endeavours to learn complex systems from observed data in order to make more informed predictions and high stakes decisions under uncertainty. The Bayesian framework provides an elegant solution to such problems, however it is typically far more expensive to compute than its deterministic counterparts. In the 21st century, and increasingly over the past decade, a growing number of methods have emerged which allow one to leverage cheap low-fidelity models in order to precondition algorithms for performing inference with more expensive models and make Bayesian inference tractable in the context of high-dimensional and expensive models. Some notable examples are multilevel Monte Carlo (MLMC), multi-index Monte Carlo (MIMC), and their randomised counterparts (rMLMC), which are able to provably achieve a dimension-independent (including infinite-dimension) canonical complexity rate with respect to mean squared error (MSE) of 1/MSE. Recently introduced double randomisation approaches deliver i.i.d. estimators of quantities of interest which are unbiased with respect to the infinite resolution target distribution and can be simulated in parallel. This talk will describe the general approach with a focus on a Markov chain Monte Carlo method. Time permitting, some sequential Monte Carlo methods will be discussed.

Sparse Online Variational Bayesian Inference

Vitaly Zankin

University of Manchester

Kody Law, University of Manchester

Minisymposium: Decision making under uncertainty

This work aims to study variational Bayesian inference for sparse regression. Sparsity promoting priors have proven to be very successful in regression scenarios since it helps to select meaningful features and avoid overfitting (e.g. LASSO regression or total variation (TV) regularization in imaging). We focus on a general class of shrinkage priors that can be represented as a scale mixture of normal distributions with a generalized inverse Gaussian distribution and includes such priors as Laplace, Generalized Jeffrey's, Student-t and others. However, since shrinkage priors are non-Gaussian, a fully Bayesian solution becomes very expensive, requiring MCMC methods. To alleviate this, we employ a variational approach that leverages a generalization of the expectation-maximization algorithm to recover the best Gaussian approximation to the sparsity-promoting posterior. This approach turns out to be especially fast and scalable in the case of linear models, where it provides approximate UQ for a substantially smaller cost than fully Bayesian approaches yet keeping comparable accuracy. Besides, the proposed approach supports online inference to process the data in batches and strategies for online hyperparameter estimation. The high performance in terms of the variable selection and UQ is demonstrated for complex real and simulated data examples where it competes against MCMC based methods as well as the other approximate approaches.

Deep Neural Networks for Inverse Problems with Pseudodifferential Operators: An Application to Limited Angle Tomography

Tatiana A. Bubba

University of Bath

Mathilde Galinier (University of Modena and Reggio Emilia), Matti Lassas (University of Helsinki), Marco Prato (University of Modena and Reggio Emilia), Luca Ratti (University of Genoa), Samuli Siltanen (University of Helsinki)

Minisymposium: Deep Learning and Inverse Problems

Sparsity promotion is a popular regularization technique for inverse problems, reflecting the prior knowledge that the exact solution is expected to have few non-vanishing components, for example, in a suitable wavelet decomposition. In this talk, I will present a novel convolutional neural network, called ΨDONet, designed for sparsity-promoting regularization for linear inverse problems. Such a network is able to replicate the application of the Iterative Soft Thresholding Algorithm (ISTA), a classical reconstruction algorithm for sparsity promoting regularization, and to actually outperform it, by learning a suitable pseudodifferential correction. By a combination of techniques and tools from regularization theory of inverse problems, multi-resolution wavelet analysis, and microlocal analysis, we are able to theoretically deduce the architecture of the network and to prove some convergence results. Our case study is limited-angle computed tomography: we test two different implementations of our network on simulated data from limited-angle geometry, achieving promising results.

A Convex Variational Model of the Blake-Zisserman Type for Segmentation of Low Contrast and Piecewise-smooth Images

Liam Burrows

University of Liverpool

Anis Theljani, Ke Chen

Minisymposium: Deep Learning and Inverse Problems

The famous Mumford-Shah model is the basis for many variational segmentation methods, though it is difficult to solve practically. Many approximations simplify the formulation by considering a piecewise-constant intensity distribution, which makes implementation easier but is usually not a realistic assumption to make for real life images. A key weakness of a piecewise-constant assumption is the lack of distinction between regions where low contrast is present.

To tackle low contrast in images, we develop a model based on the Blake-Zisserman (BZ) model which considers high order derivatives, allowing for finer edge detection. We propose a convex relaxation of the BZ model and detail how to reformulate this as a two-player Nash game. Numerical implementation is achieved via ADMM, and numerical experiments demonstrate effectiveness over similar convex models defined using various approximations of the Mumford-Shah model.

Regularising Inverse Imaging Problems Using Generative Machine Learning Models

Margaret Duff

University of Bath

Neill D F Campbell, Matthias J Ehrhardt

Minisymposium: Deep Learning and Inverse Problems

Deep neural network approaches to inverse imaging problems have produced impressive results in the last few years.

We consider the use of generative models in a variational regularisation approach to inverse problems. Generative models learn, from observations, approximations to high-dimensional data distributions. The considered regularisers penalise images that are far from the range of a generative model that has learned to produce images similar to a training dataset. We name this family generative regularisers.

In contrast to other data driven approaches, generative regularisers do not require paired training data and are learnt independently of the forward model. This makes the method very flexible in real-world scenarios where noise levels and forward model parameters may change.

In this talk I will give numerical examples demonstrating different approaches of including generative models in solving inverse problems on simple datasets. The success of these methods depends on the quality of a generator. We will discuss desired criteria for evaluating a trained generative network, in the context of inverse problems, allowing comparison between generative model approaches and providing direction for future work.

Bayesian Inference using Neural Networks As Data Driven Generative Priors

Matthew Holden

Heriot-Watt University

Marcelo Pereyra (Heriot-Watt University), Kostas Zygalakis (University of Edinburgh)

Minisymposium: Deep Learning and Inverse Problems

This talk discusses methodology for Bayesian analysis and computation in imaging inverse problems where the prior knowledge is available in the form of training data. We consider this data to be a sample from the marginal distribution of the unknown image we seek to reconstruct. Following the manifold hypothesis, and adopting a generative modelling approach, we construct a data-driven prior which can be learnt from the training data using modern machine learning techniques. We study theoretical aspects of the resulting posterior distribution (e.g., existence and well-posedness) and then propose scalable sampling algorithms to perform inference for these problems. The proposed approach is demonstrated with a range of challenging imaging problems and comparisons with alternative approaches from the state of the art. The accuracy of the prior is investigated through experiments which illustrate the benefits of a Bayesian, sampling-based approach.

Imaging conductivity from current density magnitude via neural networks

Bangti Jin
University College London
Xiyao Li, Xiliang Lu

Minisymposium: Deep Learning and Inverse Problems

Conductivity imaging represents one of the most important tasks in medical imaging. In this talk we discuss a neural network-based technique for imaging the conductivity from the magnitude of the internal current density. It is achieved by formulating the problem as the relaxed weighted least-gradient problem, and then approximating the minimizer by standard feedforward neural networks. We derive bounds on two components of the generalization error, i.e., approximation error and statistical error, explicitly in terms of properties of the neural networks (i.e., depth, total number of parameters, and the bound of the network parameters). We illustrate the performance and distinct features of the proposed approach on several numerical experiments.

Mode-2 internal solitary waves to a three-layer system

Alex Doak
University of Bath

Minisymposium: Dispersive hydrodynamics and applications

Internal waves occur in stratified fluids, such as the worlds oceans. They are responsible for the transport of momentum, heat, and organic material, as well as inducing turbulent mixing. Rather than attempting to model a continuously stratified fluid, a common simplification is to assume several homogenous layers of immiscible fluids, separated by infinitesimal interfaces. Two-layer flows have been explored extensively, and such models are used to predict wave properties of 'mode-1' waves. To explore higher modes, one needs additional interfaces. In this talk we shall discuss travelling wave solutions to a three-layer model. We will be presenting numerical solutions to both the full Euler system, and a reduced model called the three-layer Miyata-Choi-Camassa (MCC3) equations. Mode-2 waves (typically) occur within the linear spectrum, and are hence associated with a resonant mode-1 oscillatory tail. However, in line with numerical results for the MCC3 system by Barros et. al (2020), we will present numerical evidence that these oscillations can be found to have zero amplitude, resulting in a truly localised structure known as an embedded solitary wave. We also find mode-2 waves which travel faster than the maximum linear mode-1 wave speed, and are hence outside the linear spectrum. We relate large amplitude solutions to the so-called conjugate states of the system, where the limiting solutions of many of the solution branches are a heteroclinic orbit between conjugate states (i.e. wavefront solutions)

Dispersive hydrodynamics of soliton condensates

Gennady El

Northumbria University

Thibault Congy (Northumbria University), Giacomo Roberti (Northumbria University), Alexander Tovbis (University of Central Florida)

Minisymposium: Dispersive hydrodynamics and applications

We consider large-scale dynamics of non-equilibrium soliton gas of the Korteweg-de Vries (KdV) equation described by the integro-differential kinetic equation for the spectral density of states. We show that in the special "condensate" limit the spectral kinetic equation reduces to the N-phase Whitham modulation equations derived by Flaschka, Forest and McLaughlin (1980). We consider Riemann problems for the soliton condensates and identify the resulting dynamics with generalised rarefaction and dispersive shock waves. We also present numerical results for "diluted" soliton condensates exhibiting rich incoherent dispersive hydrodynamic behaviours associated with integrable turbulence.

The Interaction of Internal Solitary Waves and Sea Ice in the laboratory

Sam Hartharn-Evans

School of Mathematics, Statistics and Physics, Newcastle University

Magda Carr, School of Mathematics, Statistics and Physics, Newcastle University

Minisymposium: Dispersive hydrodynamics and applications

Internal Waves are commonly observed along density interfaces across the world's oceans. In the Arctic Ocean, the internal wave field is much less energetic than at lower latitudes, but due to relative quiescence of the region, nonlinear internal waves are particularly important for mixing there. This mixing is responsible for bringing heat from warm Atlantic Water at intermediate depth towards the surface where it has ramifications for the formation and melt of sea ice, as well as the general circulation of the Arctic Ocean. In the rapidly changing Arctic Ocean, as sea ice extent declines, understanding how internal waves interact with sea ice, and how sea ice affects them is crucial, particularly in the marginal ice zone.

Using laboratory experiments of internal solitary waves (ISWs) propagating under model ice the interaction of ice and internal solitary waves is investigated. Particle Tracking Velocimetry is used to measure the motion of floating polystyrene discs (with the same density as sea ice $\rho = 910kg/m^3$). The motion of these discs is compared to the output of numerical models, in order to quantify how ice moves in response to the near-surface internal wave-induced flow. Particle Image Velocimetry is then used to determine how the near-surface internal wave-induced flow dynamics are impacted by the presence and motion of the model sea-ice, which acts as a rough upper boundary condition and moves with the flow.

Linear stability spectra of a novel long wave-short wave system

Marcos Caso-Huerta

Northumbria University

Antonio Degasperis (Università di Roma 'La Sapienza'), Sara Lombardo (Loughborough University) and Matteo Sommacal (Northumbria University)

Minisymposium: Dispersive hydrodynamics and applications

Several integrable models have been proposed throughout the years to describe the interaction between long and short waves, among which the so-called Yajima-Oikawa and Newell models are possibly the most prominent. In this talk, a new, more general, integrable long wave-short wave model is proposed, encompassing the aforementioned systems as particular choices of the coefficients. The linear stability of plane waves for this novel system is carried out following the algebraic method proposed by Degasperis, Lombardo & Sommacal (2018), previously applied to study the vector NLS system. The Lax pair is obtained and employed to construct the locally perturbed plane wave solutions. The instabilities are investigated and classified with respect to the whole parameters space, which includes parameters featured by the system and by the solutions. The stability spectra and the associated eigenfrequencies are explicitly computed, leading to identifying a relation between the topology of the spectra and the gain of the system. Preliminary analysis indicates that, similarly to the vector NLS case, the classification of the stability spectra allows one to predict regions of existence for rogue wave type solutions.

Stability of waves on deep water with a constant background shear field

Emilian Parau

University of East Anglia

Mark Blyth, UEA

Minisymposium: Dispersive hydrodynamics and applications

The stability of periodic travelling waves on fluid of infinite depth is examined in the presence of a constant background shear field. The effects of gravity and surface tension are ignored. Linear growth rates are calculated using both an asymptotic approach valid for small amplitude waves and a numerical approach based on a collocation method. Both superharmonic and subharmonic perturbations are considered.

Undular bores governed by the full water wave equations and Whitham-Boussinesq equations.

Rosa Maria Vargas-Magana

UNAM-PAPIIT and SMM

Noel F. Smyth (University of Edinburgh) and Tim Marchant (University of Melbourne)

Minisymposium: Dispersive hydrodynamics and applications

The Dispersive Shock Fitting method, initially formulated by G. El and collaborators and later generalized to many other systems, has been applied with great success to study dispersive shock waves (DSWs) in large a variety of settings. DSWs are a generic type of wave arising as solutions of nonlinear dispersive wave equations that consist of two edges, the harmonic wave edge and solitary wave edge propagating with different speeds, with a modulated dispersive wavetrain between these. Until recently, however, most studies were limited to weakly non-linear systems. This talk aims to present our recent analytical and numerical results on DSW solutions, also termed undular bores in fluid mechanics terminology, in the context of the fully nonlinear water wave equations and four weakly nonlinear approximations to the water wave equations, including Boussinesq-type models and Whitham-Boussinesq-type models. This is joint work with Prof. Noel Smyth of the University of Edinburgh and Prof. Tim Marchant of the University of Melbourne. It is found that the Whitham-Boussinesq systems give solutions in near-perfect agreement with numerical solutions of the water wave equations for the positions of the leading and trailing edges of the bore up until the onset of modulational instability. This investigation has opened further research questions that I will also discuss in this talk

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Mathematics and ethical citizenship: Analyzing moral orders embedded in ethics and mathematics education

Sikunder Ali

Norwegian University of Science and Technology (NTNU)

Minisymposium: Ethics in Mathematics

Mathematics has been central in securing rational foundations of modern scientific enterprise. It carries with it enormous power while claiming the values of objectivity when it comes to studying/representing both physical world and mathematical worlds as often exemplified by advances in diverse computing power that is ubiquitous in our modern world. Moreover, mathematics as-a-realized-world has also been implicated in the social, economic, political, business and military world. This powerful positioning of mathematics embedded in nexus of science/technology and alignment of forces regulating and transforming social world has brought many ethical implications for social justice and ethical citizenship. That is mathematics-as-realized-world has created variety of moral orders that shape conduct of people, governments, businesses. In this context, this contribution will outline some examples of these moral orders that mathematics as-a-realized-world are creating a certain kind of picture or representation of the world and how these moral orders through these representations are bringing implications for education of mathematics at different levels of schooling. Here ethical citizenship is offered as a response to bringing critical checks to variety of powerful infrastructures that this mathematics-as-a realized world is continuously enacting with a great speed.

Hard Conversations and Consequences: Updating and Assessing the Ethical Guidelines in Mathematics

Catherine A. Buell

Fitchburg State University

Victor Piercey, Ferris State University and Rochelle Tractenberg, Georgetown University

Minisymposium: Ethics in Mathematics

The conversations around 'ethics in mathematics' are simultaneously divisive and fundamental necessary for the field. More important is connecting the theory and practice–the conversations with action. Here, progress has stagnated beyond early adopters. In true mathematical fashion, we believe a potential place for forward motion is establishing an agreement on what is true, necessary, and sufficient regarding the ethical practice of mathematics. Many mathematics professional societies have ethics codes, but they are often incomplete and only address a narrow range of mathematical practices. Mathematics practitioners need ethical guidelines that are accessible, authentic, and usable, and which reflect the community's sense of professional identity, culture of practice, and obligations to peers and the public. This can be a place to ground ethical practice to rebuild our institutions.

In this talk, we will describe the results of a recent survey of mathematical practitioners regarding the applicability of ethical provisions from various mathematics-adjacent professions to mathematics. We will highlight those items which displayed the broadest agreement, and disagreement, as touchstones for further discussion. Additionally, we will look at current trends in U.S. ethical discussions from major societies and applied maths.

A Hippocratic Oath for Mathematicians; necessary, but not sufficient

Maurice Chiodo

King's College, University of Cambridge

Dennis Mller (RWTH Aachen University), James Franklin (University of New South Wales, Sydney)

Minisymposium: Ethics in Mathematics

Early discussions about ethics, codes of conduct, or oaths, for various subdisciplines in mathematics (e.g. statistics, operations research) date back to the 1950s. The first public calls for a Hippocratic Oath for (all) mathematicians came about in the 1980s and have appeared somewhat semi-regularly ever since. But how effective have such calls been? How relevant and transferable is the Hippocratic Oath in medicine for mathematicians and their work, and how far will simply having a Hippocratic Oath go in terms of changing the actions and behaviour of mathematicians? In this talk I will give a brief survey of the various calls for a Hippocratic Oath for Mathematicians made throughout the decades. I will then examine the Hippocratic Oath in medicine, and outline why it cannot be imported directly to mathematics, neither in detail nor in structure, due to the extremely different natures of the two disciplines. This will be followed by an analysis of the additional cultural, regulatory, and professional, infrastructure that surrounds the medical profession and which gives ”teeth” to their Hippocratic Oath. I conclude by outlining the mechanisms needed in mathematics to have similar effects and give tangible support to the principles that might be contained a Hippocratic Oath for Mathematicians. This is a joint work with Dennis Mueller and James Franklin.

The Alliance for Data Science Professionals: Building trust through standards and accreditation

Rachel Hilliam and Mathew Forshaw

The Open University and University of Newcastle

Both authors will be presenting

Minisymposium: Ethics in Mathematics

The Alliance of Data Science Professionals was created to shape professional standards within data science. Such standards are needed to ensure an ethical and well-governed approach within data science, so the public, organisations and governments can have confidence in how their data are used. Members of the Alliance include The British Computer Society (BCS), The Operational Research (OR) Society, Institute of Mathematics & its Applications (IMA), The National Physical Laboratory (NPL), Royal Statistical Society (RSS) and The Alan Turing Institute (ATI). The work has gained support from Government, where it is referenced in the National Data Strategy.

While the skills of data scientists are increasingly in demand, there is currently no professional framework for those working in the field. Since the start of 2020, the Alliance has been working with volunteers and stakeholders to develop standards and competencies for individuals and standards for universities and training providers seeking accreditation of their courses. By developing a certification process and creating a single searchable public register of certified data science professionals, the Alliance will enable both individuals and education providers to gain recognition based on skills and knowledge within data science.

Twinned with the standardisation efforts of the Alliance is a commitment to support quality enhancement of data science education in the UK and internationally. Alongside The Alan Turing Institute, the Alliance is working to stimulate the development of open-source curricula addressing the most significant curricular gaps in data science and provide training to support data science educators to adopt evidence-led best practices in their delivery. For example, Anaconda, in The State of Data Science 2020, found only 15% of data science University graduates believed they had received adequate ethics training. The Alliance will support the adoption of best-in-class training to empower our professionals to protect against creating exclusionary experiences and discriminatory practices.

These new industry-wide standards seek to address current issues, such as data breaches, data misuse in modelling and bias in artificial intelligence. They can give people confidence that their data is being used ethically, stored safely, and analysed robustly.

We would like to present how the Alliance aims to achieve its goal and provide you with an opportunity to ask questions and provide feedback on the developing process.

Epidemics, ethics and uncertainty: the roles of statistics versus mathematics

Jane L Hutton

Department of Statistics, The University of Warwick

Minisymposium: Ethics in Mathematics

A few mathematicians have had considerable influence in the last two years over whether people lived and flourished, or died. Some mathematicians have focussed on designing and implementing mathematical models which only consider a single illness. Applied statisticians know that it is critical to first decide what the question is: "Minimise deaths from Covid-19?" or "Minimise deaths due to Covid-19 and our decisions this year?" or "Minimise the impact of Covid-19 on well-being over ten years?" The ethical status of an expert who gives a simple answer to the first question, without uncertainty or alternatives, will be examined.

Some publications by influential mathematics groups were directly misleading: in estimating cases of Covid-19, the assumption, made by prominent mathematicians, that PCR test had sensitivity of effectively 100%, and specificity of 80-90%, relied on gross misreading of the references cited. People were placed under effect house arrest, when, on balance of probability, they were innocent of covid.

Numbers of "covid" hospitalisations and deaths were quoted without reference to the usual daily numbers, and contributed to created a climate of fear. Predictions of 6,000 UK hospital admissions per day in January 2022 relied on the assumption that South African scientists are incompetent. Their statement that omicron variant of covid-19 has much lower admission and death rates was ignore. I will discuss whether this can be construed as racism, and compare the issues with ideas of racial inequity in UK covid death rates.

The uncertainty in diagnostic tests, missing information and measurement errors all feed into transmitted variation. Even in manufacturing glass beads, the variation from engineering specification is not simply determined by considering width, for example, alone. Despite this, mathematical predictions of covid cases were used to justify lockdowns even in countries where people would starve as a consequence. Some statisticians have tried to estimate the damage to children's education and wellbeing, and illness and deaths due to lack of access.

I argue that such mathematical modelling cannot be justified within virtue, deontological, utilitarian or care ethics. It is always necessary to consider the wider context, and the probable consequences of actions, as explained in the International Statistics Institute Code of Professional Ethics. Assessment of the validity of model assumptions, data quality, adequacy of the fit of models and accuracy of predictions is essential, and essentially statistical.

The influence of Calvin's theology on the emergence of mathematical probability and its ethical implications

Timothy Johnson
Heriot-Watt University

Minisymposium: Ethics in Mathematics

The stimulus for the emergence of mathematical probability has been obscure. Hacking argues that there was a shift in thinking in the seventeenth century but is unclear about what stimulated the shift (others, such as Franklin, deny there was any change in thinking). I will argue that the shift came out of Calvin's theology which led to a synthesis of "Stoic determinism" and "Epicurean radical uncertainty" that enabled the generalisation of chance events into general models. This genesis has interesting ethical implications, and I will highlight the Bernoulli-d'Alembert disagreement on vaccination, which is still relevant today.

On epistemic exclusion in the production of mathematical knowledge

Colin Jakob Rittberg
Vrije Universiteit Amsterdam

Minisymposium: Ethics in Mathematics

It is unsurprising that ethical issues, such as leaky pipelines or academic nepotism, arise in the social practice mathematics. In this talk I argue that some of these ethical issues impact the production of mathematical knowledge. A core insight is that having a rigorous proof of a mathematical statement is not enough. People need to be aware that you have this proof, and they need to choose to pay attention to your work. Questions about which pieces of knowledge we are exposed to and choose to engage with are entangled with issues of social power and epistemic exclusion. The production of mathematical knowledge is thus not a fully rigorous activity.

Aren't the laws of physics the same for everyone? Exploring the ethics of modelling and simulation

Erica Thompson

LSE Data Science Institute and London Mathematical Laboratory

Minisymposium: Ethics in Mathematics

Mathematical models have been in the news a lot recently. From the progress of the Covid-19 pandemic to forecasts of climate change impacts and the economic effects of Brexit, the uncertain future is made accessible to us through mathematical models. I will talk about the ethics of modelling and simulation from the mathematician's perspective. Even if the laws of physics are a separate immutable truth, the way we choose to represent them is influenced by social and political contexts. I will demonstrate that scientific and statistical choices about model construction and evaluation inevitably reflect social values, and discuss how we can make these choices responsibly. Communication of the results of modelling studies has been controversial recently; my view is that the relationship of science with society would be improved if modellers were to approach more carefully the necessity for both clarity and accountability when reporting modelled results. There are obvious corollaries for the potential role of Artificial Intelligence or autonomous systems in decision making.

Inflammation- and stress- driven airway remodelling in asthma

Bindi S Brook

University of Nottiingham

Michael R. Hill, Christopher J. Philp, Charlotte K. Billington, Amanda L. Tatler, Simon R. Johnson, Reuben D. O'Dea

Minisymposium: Inflammation and the Immune Response

Inflammation, airway hyper-responsiveness and airway remodelling are well-established hallmarks of asthma, but their inter-relationships remain elusive. In order to obtain a better understanding of their inter-dependence, we develop a mechanochemical morphoelastic model of the airway wall accounting for local volume changes in airway smooth muscle (ASM) and extracellular matrix in response to transient inflammatory or contractile agonist challenges. We use constrained mixture theory, together with a multiplicative decomposition of growth from the elastic deformation, to model the airway wall as a nonlinear fibre-reinforced elastic cylinder. Local contractile agonist drives ASM cell contraction, generating mechanical stresses in the tissue that drive further release of mitogenic mediators and contractile agonists via underlying mechanotransductive signalling pathways. Our model predictions are consistent with previously described inflammation-induced remodelling within an axisymmetric airway geometry. Additionally, our simulations reveal novel mechanotransductive feedback by which hyper-responsive airways exhibit increased remodelling, for example, via stress-induced release of pro-mitogenic and pro- contractile cytokines. Simulation results also reveal emergence of a persistent contractile tone observed in asthmatics, via either a pathological mechanotransductive feedback loop, a failure to clear agonists from the tissue, or a combination of both. Furthermore, we identify various parameter combinations that may contribute to the existence of different asthma phenotypes, and we illustrate a combination of factors which may predispose severe asthmatics to fatal bronchospasms.

Agent-based modelling of macrophage phenotype plasticity facilitating tumour cell intravasation

Joshua Bull

Wolfson Centre for Mathematical Biology, Mathematical Institute, University of Oxford

Helen Byrne, Wolfson Centre for Mathematical Biology, Mathematical Institute, University of Oxford

Minisymposium: Inflammation and the Immune Response

Macrophages are immune cells which are recruited in large numbers to damaged tissue, and constitute an important part of the immune response to tumour growth. They can display distinct phenotypes depending on microenvironmental cues. Anti-tumour M_1' macrophages are involved in tumour suppression, attacking tumour cells directly through phagocytosis and through production of inflammatory factors, which recruit a wider immune response. On the other hand, pro-tumour M_2' macrophages are implicated in immune suppression. In reality, these categories are part of a spectrum of macrophage phenotypes, with the behaviour of a particular cell being determined by the balance of cytokines it is exposed to within its local environment.

We present an agent-based model of macrophage interaction with a growing tumour. In contrast to earlier models, macrophage behaviour is determined via a continuous phenotype variable which moves along a spectrum in response to the local concentration of tumour-derived cytokines. This variable influences the sensitivity of macrophages to different chemotactic gradients, their rate of phagocytosis, and their production of EGF, a tumour cell chemoattractant. Our model reproduces a range of complex spatial patterns observed in vivo. In particular, macrophages are recruited to attack the tumour mass with an M_1-like phenotype, but once exposed to tumour-derived cytokines they gradually become more M_2-like. These cells leave the tumour mass and become perivascular macrophages, simultaneously drawing tumour cells to the vasculature through EGF production. We explore mechanisms through which tumour cells affect macrophage phenotypes, and how these phenotypes in turn affect the localisation of tumour cells.

We post-process the output from model simulations to generate four types of synthetic dataset which mimic those that can be collected from biological experiments: raw cell counts (non-spatial, no phenotype information), immunohistochemistry (spatially resolved, no phenotype information), single-cell sequencing (non-spatial, detailed phenotyping) and imaging mass cytometry (spatially resolved, detailed phenotyping). We show that different imaging techniques are suitable for describing different aspects of the biology, and that care must be taken in the selection of relevant summary statistics which describe spatial and phenotypic data in order to accurately identify simulation behaviour. Finally, we demonstrate how novel spatial statistics can be used to accurately summarise the localisation of macrophages with different phenotypes relative to vasculature and tumour cells.

Modelling the metabolism of DHA

Susan Franks

University of Nottingham

S. Preston (U. of Nottingham), V. Chapman (U. of Nottingham), P. Gowler (U. of Nottingham), J. Turnbull (U. of Nottingham), J. Dunster (U. of Reading)

Minisymposium: Inflammation and the Immune Response

Chronic pain is a major cause of disability and suffering in osteoarthritis (OA) patients. Specialised endogenous pro-resolving molecules curtail inflammatory responses, and one of the intermediate lipid mediators (17-HDHA, a metabolite of docosahexaenoic acid (DHA)) has been shown to be significantly associated with pain. We therefore develop a mathematical model to describe the metabolism of DHA using experimental data from clinical studies to ascertain how differences in the enzymatic pathways affect the associated bioactive metabolites, in particular DHA, 17-HDHA and 14-HDHA.

The law of mass action is used to generate a system of ordinary differential equations which characterise the time evolution of the concentration of bioactive lipids, dependent upon the expression of genes associated with the enzymes that metabolise the lipids. We explore the challenges and limitations of modelling real data and also discuss additional experimental data that would be useful in such modelling problems.

Pattern Formation and Transition to Chaos in a Chemotaxis Model of Inflammation

Valeria Giunta

University of Sheffield

M. C. Lombardo, University of Palermo - M. Sammartino, University of Palermo

Minisymposium: Inflammation and the Immune Response

Inflammation is a process that the immune system activates in the presence of trauma, pathogens or damaged cells. It is a protective mechanism, aiming to promptly eliminate harmful agents, remove damaged tissue and promote complete healing. However, when the immune response fails to eliminate the triggering cause or when it is determined by internal factors, as in the case of autoimmune reactions, the inflammatory process may damage healthy tissues and promote the development of diseases, often serious and debilitating such as cancer, diabetes and Multiple Sclerosis. There are different types of inflammation, which are characterized on the basis of localization or symptoms, but all share the same mechanisms, notably complex and not yet fully known. A complete and in-depth knowledge of inflammatory mechanisms therefore represents the key to the prevention and control of many diseases. In this talk, we shall present a Reaction-Diffusion-Chemotaxis system modeling the early stages the inflammatory process. Using realistic values of the parameters, we will perform a theoretical and numerical investigation of model aiming to explore the mechanisms of the immune response. First, we will analyze the occurrence of both Turing (stationary) and wave (oscillatory in time) instabilities generating spatial pattern solutions, which are able to replicate localized zones of inflammation, stationary or recurrent in time, usually observed in the clinical practice. Then, we will determine the amplitude and the shape of the supported patterns through a nonlinear analysis, with a particular focus on radially symmetric patterns, with the aim of classifying those solutions that qualitatively reproduce the formation ring-shaped skin eruptions, typically observed in patients affected by Erithema Annulare Centrifugum. Finally, we will perform a numerical bifurcation analysis far from the instability threshold and show that the model displays sequences of bifurcations leading to complex spatio-temporal dynamics, resembling the critical behaviours of immune cells. These results suggest that the proposed model, while resorting to a simplified description of the real biological system, is able to capture the key mechanisms of the inflammatory process and to provide suggestions for intervention and treatment strategies.

Mechanistic modelling towards designing personalised treatment strategies for eczema

Reiko Tanaka

Department of Bioengineering, Imperial College London

Minisymposium: Inflammation and the Immune Response

Atopic dermatitis (or eczema, AD) is the most common inflammatory skin disease, which is characterised by inflamed, dry and itchy skin leading to substantial quality of life impairment and significant socioeconomic impact. Designing personalised treatment strategies for AD is challenging, given the apparent unpredictability and large variation in AD symptoms and treatment responses within and across individuals. A first step toward developing personalised treatment strategies is to better predict the consequences of possible treatments at an individual level, rather than at population level, to deal with the variability across patients.

We developed a mechanistic model of AD pathogenesis which provided a coherent mechanistic explanation of the dynamic onset, progression, and prevention of AD, as a result of interactions between skin barrier, immune responses and environmental stressors. Model predictive control using the mechanistic model suggested a possibility for designing personalized treatment strategies. We also adapted the structure of the mechanistic model to real patient data and developed a Bayesian mechanistic model tailored to each individual, that can predict the next day's AD severity score given their score and treatments used on that day.

These works presented hopes and challenges in designing personalized treatment strategies for AD, for which detailed dynamic data is not often available.

Dissecting the cell behaviours driving inflammation and tissue repair through in vivo live imaging, genetics and computational modelling

Helen Weavers

University of Bristol

Minisymposium: Inflammation and the Immune Response

Tissues (such as the skin) must have robust strategies to rapidly repair themselves following injury. Tissue damage is normally accompanied by an inflammatory response that not only fights infection and clears debris, but also helps orchestrate the repair process. A better understanding of the molecular and cellular mechanisms controlling tissue repair and inflammation is crucial to identify therapeutic strategies for individuals suffering from chronic wound healing and inflammatory pathologies. In our studies, we dissect the various cell behaviours and signals that contribute to these processes by integrating high resolution live 4D in vivo imaging, genetic manipulation and mathematical modelling. For example, we employ a variety of computational tools to understand how immune cells behave both during homeostatic tissue patrolling and in response to tissue damage. We have previously used Bayesian modelling to uncover novel details of the pro-inflammatory attractants that draw immune cells to sites of damage. We are now extending our analysis to understand the cell behaviours that drive re-epithelialisation during wound repair and how these are influenced by the associated inflammatory response; for this, we implement cutting-edge deep learning tools as well as continuum models to extract information from our imaging datasets. Crucially, we take an iterative approach, ensuring our computational models are predictive and inform our experimental studies. Finally, we gain further insight into the factors governing tissue repair and inflammation (particularly those relevant to human health) through bespoke analysis of human genetic epidemiology data.

Supervised learning for mean field consensus control

Sara Bicego
Imperial College London
Dante Kalise (ICL), Giacomo Albi (UNIVR)

Minisymposium: Mathematical Modelling in the Social Sciences

Social behaviors can be seen as the result of a suitable combination of with-in population interactions and external influences. How to successfully condition the population towards a designed purpose (e.g. consensus) is a fascinating question, whose answer is being widely researched.

The formulation of such a problem in Optimal Control settings ensures the availability of powerful tools, which nonetheless come with the huge drawback of the curse of dimensionality. The problem reads as the minimization of a cost functional subject to individual-based interaction dynamics, thus its solution easily becomes unfeasible to reach as the number of agents in the population grows. The natural way of circumventing this is by passing from a microscopic viewpoint to a macroscopic one, from an agent-to-agent descriptions to the evolution of the population as a whole. For a number $N \to \infty$ of interacting agents, this leads to a mean field formulation of the control problem.

Although mean field optimal control problems are designed to be independent of the number N of agents, they are feasible to solve only for moderate intrinsic dimensions d of the agents' space $\Omega \in R^d$. For this reason, the solution is approached from suboptimality by means of a Boltzmann procedure, i.e. quasi-invariant limit of binary interactions as approximation of the mean field PDE, governing the dynamics of the probability distribution of the agent population. The need for an efficient solver of the binary interaction problem motivates the resorting to a supervised learning approach. As a model, we rely on a gradient augmented feedforward neural network for the Value function of the problem. The effectiveness of such a model, which has already been extensively discussed and tested, is further strengthened by the physical knowledge we hold about the phenomenon. To support the proposed methodology, numerical tests will be presented.

Bounded Confidence Models of Opinion Dynamics

Benjamin Goddard
University of Edinburgh
Beth Gooding (University of Edinburgh), Greg Pavliotis (Imperial College London), and Hannah Short (University of Edinburgh)

Minisymposium: Mathematical Modelling in the Social Sciences

This talk will focus on 'bounded confidence' models of opinions, in which people only take into account the opinion of others if they are sufficiently close in 'opinion space' (i.e. they already somewhat agree on a topic). I will first introduce agent-based, ODE, SDE, and PDE models for these dynamics, before focusing on the (nonlocal, nonlinear) PDE case, which has analogues with approaches used in statistical mechanics. The main focus of the talk will be on the complex dynamics that arise; the presence of 'phase transitions' under varying parameters in the model; the crucial choice of boundary conditions; and the introduction of 'radicals', whose opinion is invariant and act as an 'external potential'.

Parameter Estimation for Macroscopic Pedestrian Dynamics Models from Microscopic Data

Susana Gomes

University of Warwick

Andrew Stuart (Caltech) and Marie-Therese Wolfram (Warwick)

Minisymposium: Mathematical Modelling in the Social Sciences

In this talk I will present a framework for estimating parameters in macroscopic models for crowd dynamics using data from individual trajectories. I 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. I 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, I discuss possible generalisations, including the effect of the form of the fundamental diagram and the use of experimental data.

The Imagined Electorate: The role of subjective perception and objective difference in modelling vote choice

Ailsa Henderson

University of Edinburgh

Minisymposium: Mathematical Modelling in the Social Sciences

Voters in the UK believe themselves to live in nations that possess distinct values. These distinct values often include support for near universal values (support for democracy or fairness) and a perceived position on the left-right axis that marked the territory or sub-state nation as distinct. Frequently, these perceived differences are not reflected in the value profiles of these same territories. Drawing on original data this paper examines the relationship between perceived difference and actual difference to identify which experts a greater impact on vote choice across the UK. It tracks where electorates in Scotland, Wales, Northern Ireland and England perceive themselves and others to be, and also examines whether the perceived distinctiveness comes from a misrepresentation of the territory's own value profile or those of neighbours. It then explores the independent impact of self perception, group perception, and observable value profiles to see whether perception or reality experts a greater impact on vote choice.

Consensus-based models for global and multi-objective optimisation

Claudia Totzeck
University of Wuppertal

Minisymposium: Mathematical Modelling in the Social Sciences

We discuss an interacting particle dynamics modelled to find global minimisers of non-convex functions with a multitude of local minima. Besides the main ideas of the Consensus-based optimisation method, we will see recent advances for problems with high-dimensional or constrained state spaces. Theoretical results will be accompanied by numerical studies. If time permits we shed some light on a variant tailored for multi-objective problems.

Modelling the effects of deep brain stimulation in Parkinson's disease

Rafal Bogacz
University of Oxford
Gihan Weerasinghe (Oxford), Benoit Duchet (Oxford), Christian Bick (Amsterdam)

Minisymposium: Mathematical modelling of biological oscillations

Many symptoms of Parkinson's disease are connected with abnormally high levels of synchrony in neural activity. A successful and established treatment for a drug-resistant form of the disease involves electrical stimulation of brain areas affected by the disease, which has been shown to desynchronize neural activity. Recently, a closed-loop deep brain stimulation has been developed, in which the provided stimulation depends on the amplitude or phase of oscillations that are monitored in patient's brain. The aim of this work was to develop a mathematical model that can capture experimentally observed effects of closed-loop deep brain stimulation, and suggest how the stimulation should be delivered on the basis of the ongoing activity to best desynchronize the neurons. We studied a simple model, in which individual neurons were described as coupled oscillators. We first analysed the effects of stimulations through a single electrode in the model, and compared them with experimental data. Then we analysed a more general case of stimulations with electrodes including multiple contacts that can be independently controlled. Our work suggests efficient control strategies for such multi-contact closed loop deep brain stimulation.

Thalamo-Cortical Networks: Reduction, Analysis, and Modulation

Stephen Coombes

School of Mathematical Sciences, University of Nottingham

Michael Forrester and Reuben O'Dea, School of Mathematical Sciences, University of Nottingham

Minisymposium: Mathematical modelling of biological oscillations

The thalamus is a body of neural cells that relays impulses to the cerebral cortex from the sensory pathways. Feedback from the cortex gives rise to thalamo-cortical loops that generate emergent brain rhythms from the interplay of single cell ionic currents and network mechanisms. Here we discuss parsimonious models of cortex and thalamus using different types of nonlinear integrate-and-fire unit. The integrate-and-fire-or-burst model is a natural choice for building a model thalamus (from networks of relay and reticular cells) that can intrinsically oscillate via post-inhibitory rebound (mediated by a slow T-type calcium current) whilst the cortex can be more simply modelled using a network of quadratic integrate-and-fire neurons. In both cases we discuss the reduction to a lower dimensional mean-field model, utilising a separation of time-scales argument for slow synaptic interactions in the thalamus model, and the Ott-Antonsen ansatz for the cortical model. The resulting firing rate equations for both brain organs are coupled to form a thalamo-cortical loop model. The relevance of this model for understanding brain response to sensory drive is highlighted with a comparison to human neuroimaging data for median nerve stimulation.

Dynamic switching of lateral inhibition spatial patterns for cell-cell interactions

Paul Glendinning

School of Mathematics, University of Manchester, Manchester M13 9PL

Joshua Hawley, Faculty of Biology, Medicine and Health, University of Manchester, Manchester M13 9PL and N. Papadopulu Lab, Faculty of Biology, Medicine and Health, University of Manchester, Manchester M13 9PL

Minisymposium: Mathematical modelling of biological oscillations

Lateral inhibition patterns associated with Notch-Delta signalling are typically 'salt and pepper' configurations where high gene expression in one cell forces neighbouring cells into low expression. Recently a more extended non-stationary spatial pattern has been reported in developing neural tube progenitors expressing Hes5 which we are unable to model using standard nearest neighbour interactions. We describe a modified mathematical model of multicellular Hes5 expression coupled by lateral inhibition which uses internal and external noise to disrupt lateral inhibition patterns. This model has robust regions of parameter space with both dynamic switching in high/low gene expression and a noisy spatial pattern across the tissue as observed in the experiments of the Nancy Papadopulu Lab in Manchester.

Modelling the circadian clock

Hanspeter Herzel
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Minisymposium: Mathematical modelling of biological oscillations

Circadian rhythms are generated by gene-regulatory feedback loops in virtually all mammalian cells. The intrinsic clock orchestrates physiology, metabolism, and activity. External zeitgebers such as light, temperature and meals entrain the autonomous body clock. We present mathematical models addressing the following questions: How to achieve robust rhythms with a synergy of negative and positive feedback loops? How synchronization of cells in the brain is achieved? What controls the phase of entrainment ("chronotype")? Finally, we discuss the optimization of cancer chronotherapy.

Why do we procrastinate in going to bed and struggle to get up in the morning? Using mathematics to design light interventions to improve sleep timing

Anne C Skeldon
University of Surrey

Minisymposium: Mathematical modelling of biological oscillations

When we sleep depends on the interaction of multiple factors including our individual physiology, our light environment and work and other constraints on our time. Non-smooth coupled oscillator models that capture the essence of the underlying physiology (circadian rhythmicity and sleep homeostasis), light exposure and social constraints are important to help de-construct the relative importance of each of these factors.

In this talk I will discuss some of our recent work that aims to use mathematical models to quantitatively describe individual sleep timing. I'll illustrate how seasonal desynchrony with the 24 h day as seen in some people living with schizophrenia can be explained by changes in light and how we are combining models and data to design personalised light interventions. I'll touch on some of the challenges in modelling individual day-to-day variability in sleep timing.

Entrainment dynamics organised by global manifolds in a circadian pacemaker model

Kyle Wedgwood

University of Exeter

Jennifer Creaser (University of Exeter), Casey Diekman (New Jersey Institute of Technology)

Minisymposium: Mathematical modelling of biological oscillations

Circadian rhythms are established by the entrainment of our intrinsic body clock to periodic forcing signals provided by the external environment, primarily variation in light intensity across the day/night cycle. Loss of entrainment can cause a multitude of physiological difficulties associated with misalignment of circadian rhythms, including insomnia, excessive daytime sleepiness, gastrointestinal disturbances, and general malaise. This can occur after travel to different time zones, known as jet lag; when changing shift work patterns; or if the period of an individual's body clock is too far from the 24-hour period of environmental cycles. In this talk, we consider the loss of entrainment and the dynamics of re-entrainment in a two-dimensional variant of the Forger-Jewett-Kronauer model of the human circadian pacemaker forced by a 24-hour light/dark cycle. In particular, we explore the loss of entrainment by continuing bifurcations of one-to-one entrained orbits under variation of forcing parameters and the intrinsic clock period. We show that the severity of the loss of entrainment is dependent on the type of bifurcation inducing the change of stability of the entrained orbit, which is in turn dependent on the environmental light intensity. We further show that for certain perturbations, the model predicts a counter-intuitive rapid re-entrainment if the light intensity is sufficiently high. We explain this phenomenon via computation of invariant manifolds of fixed points of a 24-hour stroboscopic map and show how the manifolds organise re-entrainment times following transitions between day and night shift work

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From root hydraulic architectures to macroscopic representations of root hydraulics in land surface models

Valentin Couvreur

Universit catholique de Louvain

Jan Vanderborght, Flicien Meunier, Andrea Schnepf, Harry Vereecken, Martin Bouda, and Mathieu Javaux

Minisymposium: Mathematical models of plant-soil interactions

Root water uptake is an important process in the terrestrial water cycle. How this process depends on soil water content, root distributions, and root properties is a soil root hydraulic problem. We compare different approaches to implement root hydraulics in macroscopic soil water flow and land surface models. By upscaling a three-dimensional hydraulic root architecture model, we derived an exact macroscopic root hydraulic model. The macroscopic model uses the following three characteristics: the root system conductance, Krs, the standard uptake fraction,

SUF, which represents the uptake from a soil profile with a uniform hydraulic head, and a compensatory matrix that describes the redistribution of water uptake in a non-uniform hydraulic head profile. The two characteristics, Krs and SUF, are sufficient to describe the total uptake as a function of the collar and soil water potential, and water uptake redistribution does not depend on the total uptake or collar water potential. We compared the exact model with two hydraulic root models that make a priori simplifications of the hydraulic root architecture, i.e., the parallel and big root model. The parallel root model uses only two characteristics, Krs and SUF, which can be calculated directly following a bottom-up approach from the 3D hydraulic root architecture. The big root model uses more parameters than the parallel root model, but these parameters cannot be obtained straightforwardly with a bottom-up approach. The big root model was parameterized using a top-down approach, i.e., directly from root segment hydraulic properties, assuming a priori a single big root architecture. This simplification of the hydraulic root architecture led to less accurate descriptions of root water uptake than by the parallel root model. To compute root water uptake in macroscopic soil water flow and land surface models, we recommend the use of the parallel root model with Krs and SUF computed in a bottom-up approach from a known 3D root hydraulic architecture.

Lockhart with a twist: Modelling cellulose microfibril deposition and reorientation reveals twisting plant cell growth mechanisms

Rosemary J Dyson

University of Birmingham

Jeevanjyoti Chakraborty (Indian Institute of Technology Kharagpur), Jingxi Luo (University of Birmingham)

Minisymposium: Mathematical models of plant-soil interactions

Plant morphology emerges from cellular growth and structure. The turgor-driven diffuse growth of a cell can be highly anisotropic: significant longitudinally and negligible radially. Such anisotropy is ensured by cellulose microfibrils (CMF) reinforcing the cell wall in the hoop direction. To maintain the cell's integrity during growth, new wall material including CMF must be continually deposited. We develop a mathematical model representing the cell as a cylindrical pressure vessel and the cell wall as a fibre-reinforced viscous sheet, explicitly including the mechano-sensitive angle of CMF deposition and discuss our findings. The model incorporates interactions between turgor, external forces, CMF reorientation during wall extension, and matrix stiffening. Overall, this study provides a unified mechanical framework for understanding left- and right-handed twist-growth as seen in many plants.

Control models for crop management: Application to wastewater reuse

Antoine Haddon

LBE, INRAE

Jérôme Harmand (LBE, INRAE); Alain Rapaport (MISTEA, INRAE); Sébastien Roux (MISTEA, INRAE)

Minisymposium: Mathematical models of plant-soil interactions

Mathematical control theory tools are not yet widely applied to agricultural systems, although they could be used to improve the optimisation of crop management and serve as a basis for decision support tools. In particular, modern crop models are generally computer models with complex mathematical structures that limit the ability to apply efficient optimization techniques. On the other hand, decision models do not necessarily need to be as detailed as models for deep understanding of internal processes and furthermore, limited decision variables and relatively poor online measurements also advocate for simple models. In this context, the development and use of control oriented models will be presented with applications towards the reuse of wastewater for irrigation. First, it will be shown how reduced models can be used with soil water content data to deal with sensor faults and spatial variability in soil structure. Secondly, a double modelling method is proposed that allows to use in parallel a detailed crop model and a reduced order model for the resolution of optimal control problems in crop management.

Modelling the impact of root-guided preferential soil moisture flow on plant water uptake

Andrew Mair

The Maxwell Institute for Mathematical Sciences, Edinburgh

Mariya Ptashnyk (Heriot-Watt University) and Lionel Dupuy (NEIKER)

Minisymposium: Mathematical models of plant-soil interactions

Evidence exists that preferential flow (PF) of moisture through vegetated soil can be attributed to the structural traits of the plant root system that occupies it. Furthermore, it is known that these traits will also affect the spatiotemporal distribution of root water uptake (RWU). Therefore, the ability to investigate which structural root system traits induce desirable patterns of PF, and improve RWU efficiency, is of obvious worth to those involved in agriculture and land management. The aims of this work are: (i) to develop and calibrate a novel mathematical model for soil moisture transport that incorporates root-guided PF and compensatory RWU, and (ii) to use the developed model to investigate the impact of changes in root system structure on RWU, when explicitly accounting for root-guided PF. We parametrise our model using data for Maize plants grown in a silt loam soil and use Bayesian optimisation to calibrate. We use the finite-element method to provide numerical solutions to our developed model, which simulate soil moisture transport and RWU. The results of these simulations, and what they reveal regarding desirable root system traits, will form the basis of our discussion.

Crowd movement in bacteria colonisation of rhizosphere

Matthias Mimault

The James Hutton Institute

Lionel X. Dupuy, Neiker; Mariya Ptashnyk, Heriot-Watt University

Minisymposium: Mathematical models of plant-soil interactions

The migration of bacteria in the soil is a key but complex process for the establishment of microbiomes in the rhizosphere. Recent observations have revealed high degrees of cell-cell coordination and dynamic flock-like behaviour in the pore space. It has been hypothesised that such movement are driven by extracellular signals and quorum sensing, and could increase swimming efficiency, without being yet demonstrated experimentally.

Here, we propose a mathematical framework to explain this transport based on nonlocal interaction. The mathematical model indicates that the diffusion of extracellular signals alone cannot explain the formation of bacterial flocks, and that peer presence in a neighbourhood can influence the travel decisions of a bacteria. The diffusivity of the medium improves the distance of interaction, increasing the effective area of interaction and overall morphology of the flocks. These findings suggest that models for bacterial chemotaxis in soil should include more sophisticated mechanisms for cell-cell communication.

Modelling Root System Architectures in Challenging Soil Environments

Ernst Dirk Schfer

Independent

Ernst D. Schfer, Markus R. Owen (University of Nottingham), Ian Vernon (Durham University), Leah Band (University of Nottingham), Etienne Farcot (University of Nottingham), Jonathan P. Lynch (Pennsylvania State University)

Minisymposium: Mathematical models of plant-soil interactions

OpenSimRoot is a functional-structural plant model which allows us to simulate the growth and behaviour of roots in a simulated soil. OpenSimRoot has been used to simulate the utility of root traits in barley, bean, maize, rice and squash in a variety of scenarios and is under active development. Using computationally-intensive models like OpenSimRoot, searching high-dimensional parameter spaces for parameter combinations that optimise model output metrics is very challenging; we address this challenge using an emulator-based approach. We used statistical machine learning techniques to construct an emulator that is able to mimic the behaviour of OpenSimRoot with a minute fraction of the computing power OpenSimRoot requires. This allowed us to search a 17-dimensional parameter space for the maize root systems that maximised shoot growth in a soil with low nitrogen, phosphorus and potassium availability. After 4 iterations of running simulations, (re)training the emulator and selecting promising parts of parameter space we identified a region of parameter space with high-performing root systems and determined the releative importance of root system traits for explaining the variation in shoot dry weight. These results highlight the potential of statistical machine learning methods for trait optimisation in the context of biological modelling.

It's good to talk (but not too quickly): emergent robustness of bacterial conversations due to delayed bifurcations

Mohit Dalwadi

University College London

Minisymposium: Mathematics in microbiology

Bacteria use intercellular signalling, or quorum sensing, to share information and respond collectively to aspects of their surroundings. However, the autoinducers that carry this information must be exposed to the external environment in order to pass between bacteria. Consequently, these autoinducers are susceptible to removal through fluid flow, a ubiquitous feature of bacterial habitats ranging from the gut and lungs to lakes and oceans. Given that detecting local autoinducer concentration is fundamental to bacterial quorum sensing, how does bacterial communication remain robust in unsteady flow environments?

We develop and apply a general theory that identifies and quantifies the conditions required for quorum sensing activation in fluid flow by systematically linking cell- and population-level genetic and physical processes. By exploring the emergent delay dynamics across an imperfect transcritical bifurcation in the system, we predict that cell-level positive feedback promotes a robust collective response, and can act as a low-pass filter at the population level in oscillatory flow, responding only to changes over slow enough timescales. Moreover, we use our model to predict how bacterial populations can discern between increases in cell density and decreases in flow rate.

Founder cell configuration drives competitive outcome within colony biofilms

Fordyce A. Davidson

University of Dundee

Lukas Eigentler[1], Margarita Kalamara[1], Graeme Ball[1], Cait E. MacPhee[2], Nicola R. Stanley-Wall[1], Fordyce A. Davidson[1].

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Minisymposium: Mathematics in microbiology

Bacteria can form dense communities called biofilms, where cells are embedded in a self-produced extracellular matrix. Exploiting competitive interactions between strains within the biofilm context can have potential applications in biological, medical, and industrial systems. By combining mathematical modelling with experimental assays, we reveal that spatial structure and competitive dynamics within biofilms are significantly affected by the location and density of the founder cells used to inoculate the biofilm. Using a species-independent theoretical framework describing colony biofilm formation, we show that the observed spatial structure and relative strain biomass in a mature biofilm comprising two isogenic strains can be mapped directly to the geographical distributions of founder cells. Moreover, we define a predictor of competitive outcome that accurately forecasts relative abundance of strains based solely on the founder cells potential for radial expansion. Consequently, we reveal that variability of competitive outcome in biofilms inoculated at low founder density is a natural consequence of the random positioning of founding cells in the inoculum. Extension of our study to non-isogenic strains that interact through local antagonisms, shows that even for strains with different competition strengths, a race for space remains the dominant mode of competition in low founder density biofilms. Our results, verified by experimental assays using Bacillus subtilis, highlight the importance of spatial dynamics on competitive interactions within biofilms and hence to related applications.

The impact of boundaries on micro-swimmer distributions in channel flow, and the resultant boundary encounter angles

Smitha Maretvadakethope

University of Liverpool

Andrew L. Hazel (University of Manchester), Bakhti Vasiev (University of Liverpool), and Rachel N. Bearon (University of Liverpool)

Minisymposium: Mathematics in microbiology

A critical area of interest when developing medical technologies, like catheters, or when developing infrastructures, like water supply pipes, is biofilm formation, as biofilms can lead to contamination and infection risks. For motile swimming organisms, the early stages of biofilm colonization are dependent on microswimmer properties and the flow environments they are suspended in. These properties also affect the rate of surface colonisation and the effective diffusion of different microswimmers. We study the initial stages of biofilm formation for the case of a dilute suspension of microswimmers in two-dimensional pressure-driven flows. We particularly focus on the effects of swimmer geometry and linearly varying shear throughout bulk-flow on swimmer trajectories and how the history of bulk-flow dynamics affects swimmer-wall interactions. We obtain population-level features of the equilibrium problem through continuum modelling (using a two-dimensional Smoluchowski equation) and use individual-based stochastic models to analyse the observed features, explore cell behaviours throughout the flow and study the resulting swimming orientation distributions at the wall in the absence of hydrodynamic wall interactions. We determine the importance of the deterministic effects of swimming in channel flow on the swimmer orientation distribution at the channel wall via a novel accumulation index, and use individual based models to study the roles of rotational and translational diffusion on the trajectories of microswimmers interacting with the walls. We further study the interplay between the choice of different

boundary conditions in continuum modelling, and the observed bulk-flow dynamics. These insights highlight the non-triviality of the choice of boundary conditions when conducting numerical studies of microswimmer suspensions via continuum models, and the importance of shape and shear effects on swimmer-wall interactions.

Dynamics of squirmers in a confined anisotropic fluid

Marco Mazza

Loughborough University

Minisymposium: Mathematics in microbiology

We study the dynamics of a model squirmer in a nematic liquid crystal using particle-based hydrodynamic simulations (MPCD) method. A recently developed nematic fluid model [Phys. Rev. E **99**, 063319 (2019)] which employs a tensor order parameter to describe the spatial and temporal variations of the nematic order is used to simulate the surrounding anisotropic fluid. Considering both nematodynamic effects (anisotropic viscosity and elasticity) and thermal fluctuations, in the present study, we couple the nematic MPCD algorithm with a molecular dynamics (MD) scheme for the squirmer. To test the applicability of this nematic MPCD-MD method, we simulate the dynamics of a spherical squirmer with homeotropic surface anchoring conditions in a bulk domain. The importance of anisotropic viscosity and elasticity on the squirmer's speed and orientation is studied for different values of self-propulsion strength and squirmer type (pusher, puller or neutral). In sharp contrast to Newtonian fluids, the speed of the squirmer in a nematic fluid depends on the squirmer type. Interestingly, the speed of a strong pusher is smaller in the nematic fluid than for the Newtonian case. The orientational dynamics of the squirmer in the nematic fluid also shows a non-trivial dependence on the squirmer type. Our results compare well with existing experimental and numerical data.

Multiscale modelling of bacterial populations

Philip Pearce

University College London

Minisymposium: Mathematics in microbiology

Bacterial populations often exhibit collective behaviour, for example by forming biofilms or swarms. The formation and organisation of such multicellular communities is mediated by cell growth, division and motility, external forces, and physical and chemical interactions between cells. In this talk, I will demonstrate how mathematical modelling at the levels of individual cells and whole communities reveals the underlying physical principles of bacterial collective behaviour.

Novel treatment of chronic wounds using bioactive glass fibres - a partial differential equation model

Sandeep Shirgill

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Minisymposium: Mathematics in microbiology

Chronic wounds (principally pressure sores, venous leg ulcers and diabetic foot ulcers) are a drain on global health services and remain a major area of unmet clinical need. Chronic wounds are characterised by a stable and stubborn bacterial biofilm which hinders innate immune response and delays or prevents wound healing. Bioactive glass fibres, which have a cotton-wool like appearance, offer a promising treatment for chronic wounds. When fibres are placed in fluid, they undergo multiple chemical reactions such as: leeching, dissolution, and precipitation. Si4+ and Ca2+ ions are released during dissolution can promote wound healing. Fibres may also be doped with other inorganic ions, for example Ag+ and Cu2+, which are known to have antimicrobial activity. Here, an partial differential equation model is developed to investigate the sensitivity of certain parameters and identify value ranges in which a chronic wound may be healed by bioactive glass fibre treatment. Key parameters that are investigated are: ion release rates from fibres, ion potency and packing density of fibres. Experimental data gathered is used to fit certain parameters and validate the model. Model simulations suggest that for a chronic wound to be healed, any bacterial biofilm present must be eradicated as soon as possible. Furthermore, the rate of signalling molecule production by fibroblasts is a critical parameter; this rate must be sufficiently high for treatment success. Finally, the model predicts that using a combination of bioactive glass fibre treatment and debridement will be much more effective than using either bioactive glass of debridement alone.

Modelling Antibiotic Resistance Gene Spread in Wastewater Treatment Plants

Cansu Uluseker

Minisymposium: Mathematics in microbiology

Wastewater treatment plants (WWTPs) receive wastewater that carries a variety of pollutants, including antibiotics. Due to their large and diverse community of organisms, WWTPs become hot spots for antibiotic resistance genes (ARGs) and increase the spread of antibiotic-resistant bacteria (ARB). However, Effective WWTPs can act as a final barrier to prevent ARB receives to the environment. Therefore, it is important to develop a model to understand the mechanism of the ARG spread in WWTP. We developed a mathematical model that describes: 1, the spread of

antibiotic resistance genes across populations of bacteria in wastewater treatment plants; and that at the same time describes: 2, the dynamics of the activated sludge process and the biochemical removal and cycling of wastewater components

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A statistical framework for mapping context-specific regulatory variants using scRNA-seq

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Minisymposium: Mathematics in single-cell biology

Single cell RNA sequencing (scRNA-seq) enables characterizing the cellular heterogeneity in human tissues. Technological advances have enabled the first population-scale scRNA-seq studies in hundreds of individuals, allowing to assay genetic effects with single-cell resolution. However, existing strategies to perform genetic analyses using scRNA-seq remain based on principles established for bulk RNA-seq. In particular, current methods depend on a priori definitions of discrete cell types, and hence cannot assess allelic effects across subtle cell types and cell states. To address this, we propose Cell Regulatory Map (CellRegMap), a statistical framework to test for and quantify genetic effects on gene expression in individual cells. CellRegMap provides a principled approach to identify and characterize heterogeneity in allelic effects across cellular contexts of different granularity, including cell subtypes and continuous cell transitions. We validate CellRegMap using simulated data and apply it to two recent studies of differentiating iPSCs, where we uncover a previously underappreciated heterogeneity of genetic effects across cellular contexts. Finally, we identify fine-grained genetic regulation in neuronal subtypes for eQTL that are colocalized with human disease variants.

Unravelling the correlation structure of noise in molecular pathways

Lucy Ham

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Minisymposium: Mathematics in single-cell biology

Noise is ubiquitous at the molecular scale, and its presence has profoundly shaped cellular life. Understanding the sources of noise, how it is propagated, amplified, and attenuated has therefore become a cornerstone of modern cellular biophysics.

Often seen as a nuisance, we here show how the correlation structure of noise can be exploited to dissect the molecular machinery underlying cellular processes.

Noise leads to significant heterogeneity between cells subject to identical conditions, observable in snapshot distributions of molecule (e.g., transcript) numbers across ensembles of cells. Because temporal information is lost in such data, we are presented with significant challenges for inferring the molecular mechanisms underlying gene transcription, as well as the causes of cell-to-cell variability. In particular, we typically cannot separate dynamic variability from within cells ("intrinsic noise") from variability across the population ("extrinsic noise"). By developing stochastic models of gene expression that describe both intrinsic and extrinsic noise (Fig. A), we prove that it is in general impossible to identify the sources of variability, and consequently, the underlying transcription dynamics, from observed transcript abundance distributions alone. Systems with intrinsic noise alone can always present identically to similar systems with extrinsic noise.

Using these results, we identify new experimental set-ups that can assist in resolving this non-identifiability. We show that multiple generic reporters from the same biochemical pathways (e.g., mRNA and protein) can infer magnitudes of intrinsic and extrinsic transcriptional noise, identifying sources of heterogeneity (Fig. B). We validate this approach for restoring identifiability using synthetic data for genes with non-trivial gene expression dynamics; "pathway-reporter" approaches are remarkably robust to the details of the mRNA and protein synthesis dynamics. Stochastic simulations show further that pathway reporters compare favourably to the well-known, but often difficult to implement, dual-reporter methods. While experimental design has often played a subsidiary role in single-cell transcriptomics, our approach shows how the correlated structure of noise can be used to gain deeper mechanistic insights into molecular processes from snapshot data.

CellRank for directed single-cell fate mapping

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Minisymposium: Mathematics in single-cell biology

Computational trajectory inference enables the reconstruction of cell-state dynamics from single-cell RNA sequencing experiments. However, trajectory inference requires that the direction of a biological process is known, largely limiting its application to differentiating systems in normal development. Here, we present CellRank (https://cellrank.org) for single-cell fate mapping in diverse scenarios, including regeneration, reprogramming and disease, for which direction is unknown. Our approach combines the robustness of trajectory inference with directional information from RNA velocity, taking into account the gradual and stochastic nature of cellular fate decisions, as well as uncertainty in velocity vectors. On pancreas development data, CellRank automatically detects initial, intermediate and terminal populations, predicts fate potentials and visualizes continuous gene expression trends along individual lineages. Applied to lineage-traced cellular reprogramming data, predicted fate probabilities correctly recover reprogramming outcomes. CellRank also predicts a novel dedifferentiation trajectory during post-injury lung regeneration, including previously unknown intermediate cell states, which we confirm experimentally.

Modularity, criticality, and evolvability of a developmental gene regulatory network

Berta Verd

University of Oxford

Nicholas AM Monk, University of Sheffield. Johannes Jaeger, Complexity Science Hub Vienna

Minisymposium: Mathematics in single-cell biology

The existence of discrete phenotypic traits suggests that the complex regulatory processes which produce them are functionally modular. These processes are usually represented by networks. Only modular networks can be partitioned into intelligible subcircuits able to evolve relatively independently. Traditionally, functional modularity is approximated by detection of modularity in network structure. However, the correlation between structure and function is loose. Many regulatory networks exhibit modular behaviour without structural modularity. Here we partition an experimentally tractable regulatory network the gap gene system of dipteran insects using an alternative approach. We show that this system, although not structurally modular, is composed of dynamical modules driving different aspects of whole-network behaviour. All these subcircuits share the same regulatory structure, but differ in components and sensitivity to regulatory interactions. Some subcircuits are in a state of criticality, while others are not, which explains the observed differential evolvability of the various expression features in the system.

Learning to Segment Cells by Co-localizing Image Patches

Steffen Wolf

MRC Laboratory of Molecular Biology, Cambridge

Kate McDole (Laboratory of Molecular Biology), Jan Funke (HHMI Janelia Research Campus)

Minisymposium: Mathematics in single-cell biology

The segmentation of cells and objects in microscopy images is a complex image analysis problem, which often requires a human annotator to manually label images in a highly labour-intensive process. Machine learning methods seek to automate this task, however also require large amounts of manually generated training data. This talk will introduce a self-supervised learning method in order to greatly reduce the number of training examples needed for segmentation.

We propose to train neural networks on fluorescent microscopy image patches by predicting their relative location. We show how the trained networks ability to find the correct relative position of patches can be utilized to generate a segmentation without annotations. Furthermore, we show that these segmentations can supplement supervised network training and lead to a significant reduction in the number of required training annotations.

Dynamic inference from single-cell snapshots by optimal transport

Stephen Zhang

University of Melbourne (previously University of British Columbia)

Anton Afanassiev, Laura Greenstreet, Tetsuya Matsumoto, Geoffrey Schiebinger (University of British Columbia)

Minisymposium: Mathematics in single-cell biology

Understanding how cells change their identity and behaviour over time in living systems is a key question in many fields of biology. Measurement of cell states is inherently destructive, and so the relationship of the current state of a cell to some future state, or fate, cannot be observed experimentally. Trajectory inference refers to the general problem of trying to estimate various aspects of the state-fate relationship. Motivated by a diffusion-drift-growth model of single-cell dynamics, we discuss optimal transport theory as a useful analytical tool for trajectory inference. Using these tools, we develop a methodology for recovering trajectories in settings where a single-cell snapshot is observed from a population of asynchronously developing cells.

Mathematical Models of a Heterogeneous Vitreous Humour: An Investigation into Vitreoschisis and the Premacular Bursa

Laura Bevis

Imperial College London

Minisymposium: Mathematics of the eye

Retinal detachment affects around 1 in 10,000 people per year, and, since the retina is vital for vision, this can quickly lead to sight loss if left untreated. The retina lines the posterior side of the vitreous chamber at the back of the eye, which is filled with the gel-like vitreous humour. The motion of the vitreous, induced by eye movements, imposes mechanical stresses on the retina, which are thought to be the leading cause of rhegmatogenous retinal detachments.

The vitreous is spatially heterogeneous with liquefied regions in the gel. The mechanical effects of this are not clearly understood and are difficult to determine experimentally. We model two cases, the premacular bursa (thought to be an anatomical feature that protects the retina), and a vitreoschisis (occurs due to vitreous degeneration). We present several mathematical models of a fluid-filled space in the vitreous and investigate the effect of everyday oscillatory eye movements on the shear stresses felt by the retina. We model the spaces both indirectly, using a mathematical slip condition on the eye wall, and directly using boundary integral techniques. We find that the premacular bursa reduces the shear stress significantly over the macula, while the vitreoschisis significantly increases the retinal shear stress towards its edges. Most importantly, we observe a local jump in the shear stress along the retina, at the ends of the vitreoschisis, suggesting that it experiences a constant pushing and pulling there, which could lead to local retinal damage.

As well as providing information of significant clinical interest, the models presented are fundamentally interesting mathematical problems in their own right, since we make use of techniques that are more commonly used for other flow regimes.

The role of Bayesian inference in understanding Macular degeneration

Jessica Crawshaw

The Mathematical institute, University of Oxford

Eamonn Gaffney (University of Oxford), Philip Maini (University of Oxford) Antonello Caruso (The Roche Institute), Michael Gertz (The Roche Institute)

Minisymposium: Mathematics of the eye

TBC

A mathematical model of aqueous humour production

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Alexander J.E. Foss (Department of Ophthalmology, Nottingham University Hospitals NHS Trust), Eamonn A. Gaffney (Wolfson Centre for Mathematical Biology, Mathematical Institute, University of Oxford) and Rodolfo Repetto (Department of Civil, Chemical and Environmental Engineering, University of Genoa)

Minisymposium: Mathematics of the eye

Aqueous humour (AH) is a transparent water-like fluid that fills the anterior segment of the eye. It is produced by a tissue called ciliary processes, located behind the iris, where it is secreted by the ciliary epithelium (CE). It then flows through the posterior chamber of the eye (i.e. the region between the iris and the lens) and exits via the pupil into the anterior chamber (i.e. the region between the cornea and the iris), where it is drained into the trabecular meshwork. This flow is very important physiologically, as the balance between the rate of AH production and resistance to its drainage governs the intraocular pressure (IOP). Elevated IOP is correlated with the occurrence of glaucoma. Lowering AH production rate may assist in prevention or treatment of glaucoma. Therefore, understanding of underlying physical mechanisms that govern the production of AH is of great clinical relevance.

In this work we propose a mathematical model of fluid and solute transport across the CE with the aim to study mechanisms of AH production, determine how the AH production rate depends on the controlling parameters and how it can be manipulated. We employ a compartmental transport model that consists of stroma, CE and the posterior chamber, filled with the fluid and various solutes, such as ions and CO_2. We impose conservation of mass in the CE and the posterior chamber for water and each considered solute, accounting for the presence of the ion channels located on the cell membranes and reactions between the solutes.

With a feasible set of parameters the model predictions of water flux from the stroma to the posterior chamber and of the solute concentrations in the AH are in good agreement with measurements. Using global sensitivity analysis we also identify the key parameters which impact the aqueous production rate. In particular, a relevant role is predicted to be played by cell membrane permeability to potassium and chloride, as well as by the NHE channel and carbonic anhydrase. The model thus provides insight into the physical processes underlying the functioning of drugs that are adopted to regulate aqueous production. It also suggests ion channels and cell membrane properties that may be targeted to manipulate aqueous production rate.

Mathematical Models of Retinal Degeneration

Dr Paul A Roberts
University of Birmingham

Minisymposium: Mathematics of the eye

The retina is a tissue layer at the back of the eye that uses photoreceptor cells to detect light. Photoreceptors can be characterised as either rods or cones. Rods provide achromatic vision under low light conditions, while cones provide high-acuity colour vision under well-lit conditions. The term Retinitis Pigmentosa (RP) refers to a range of genetically mediated retinal diseases that cause the loss of photoreceptors and hence visual function. RP leads to a patchy degeneration of photoreceptors and typically directly affects either rods or cones, but not both. During the course of the disease, degenerate patches spread and the photoreceptor type unaffected by the mutation also begins to degenerate. The cause underlying these phenomena is currently unknown; however, several key mechanisms have been hypothesised: oxygen toxicity, trophic factor depletion and the release of toxic substances by dying cells. Here we present mathematical models, formulated as systems of PDEs, to investigate the trophic factor hypothesis. Using a combination of numerical simulations and mathematical analysis, we determine the geographic variation in retinal susceptibility to degeneration, predict the effects of various clinically-relevant treatment strategies, predict spatio-temporal patterns of degeneration and solve an inverse problem to determine the conditions under which in vivo spatio-temporal patterns of degeneration are replicated by our models.

Elastic jump propagation through retinal networks in response to trauma

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Peter S. Stewart, School of Mathematics and Statistics, University of Glasgow, UK

Minisymposium: Mathematics of the eye

A severe head impact can cause bleeding in the eye, called retinal haemorrhage. One proposed mechanism is that a blow to the head causes an increase of pressure in the cerebrospinal fluid surrounding the skull, which is imparted to the blood vessels which feed the retina (the central retinal artery and vein), through which the pressure is directly transmitted. This perturbation then induces blood vessels to burst as it travels through the retinal circulation. Here we analyse the induced disturbance, which can steepen to form an elastic jump (a feature characterised by a sudden change in vessel cross-sectional area), at the eye entrance and as it propagates through bifurcations deeper into the retina.

We model the vessels as elastic tubes containing Newtonian fluid in one spatial dimension. To account for the vessel passing through the optic nerve sheath at the entrance to the eye, we model the vessel as a multi-compartment tube, with disturbances driven by an external pressure imparted to one compartment. We use a finite volume model compared to a linear analytic model. We show that confining effects of the optic nerve sheath spread out the induced disturbance within the eye (which can be an elastic jump), reducing its amplitude. This scales inversely proportionally to the length of the confined vessel region. Hence, this confined region is having a protective effect on the eye.

Next, we analyse this elastic jump as it moves through a vessel bifurcation, consisting of one parent and two daughter vessels, imposing conservation of mass and total pressure at the junction. We prescribe the pressure of the incoming elastic jump in the parent vessel and calculate the three induced elastic jumps (one reflected back up the parent vessel and two transmitted down each daughter vessel), using our finite volume method and validated against a simpler model using Rankine-Hugoniot jump conditions. We analyse this system for increasing pressure of the incoming elastic jump and demonstrate a limit for the existence of a stable three elastic jump solution.

The Human Tear Film Modelling: Marx's line formation

Vladimir Zubkov

Wolfson College - Oxford University

C.J.W. Breward (Oxford University) and E.A. Gaffney (Oxford University)

Minisymposium: Mathematics of the eye

The first optical element of the eye is the cornea, essential for image formation and hence for sight. The exposed cornea is covered by a protective tear film, which prevents desiccation of the surface epithelia by evaporation. The tear film consists of an aqueous layer containing numerous physiological salts and a surface lipid layer. Dysfunction of the tear film gives rise to a disabling condition of the ocular surface called dry eye whose prevalence worldwide is between 12-30%. We have formulated and explored a model describing the spatial distribution of tear film osmolarity across the ocular surface of a human eye during one blink cycle, incorporating detailed fluid and solute dynamics. Based on the lubrication approximation, our model comprises three coupled partial differential equations tracking the thickness of the aqueous layer of the tear film, the concentration of the polar lipid and the concentration of physiological salts contained in the aqueous layer. We have also studied the meniscal dynamics using the Navier-Stokes equations to explore the formation of Marx's line.

Application of fluid dynamics in modelling indoor airborne disease transmission and developing mitigating strategies

Rajesh K Bhagat

Department of Applied Mathematics and Theoretical Physics

Minisymposium: Modelling the respiratory transmission of Covid-19

Throughout human history, nothing has killed more people than infectious diseases. Natural pandemics are ever-present and the next pandemic is a matter of when not if. The event frequency for pandemics caused by natural and synthetic pathogens are likely to increase due to human encroachment into natural environments, bio-terrorism threats, high population density urban settings, lifestyles, and global connectivity. Covid-19 has clearly demonstrated the lack of understanding of airborne disease transmissions: we have been caught responding too late to the situation, and there is an urgent need to develop fundamental understandings and improve preparedness at all levels.

Essentially, indoor airborne disease transmission is a fluid dynamics problem; the formation of potentially contagion laden droplet/bio-aerosols is an interfacial flow problem and their subsequent transport in the indoor environment is a building ventilation flow problem. Dealing with Covid-19 has clearly demonstrated the need for a better understanding of these problems and, most importantly, dissemination of existing knowledge for their real-world application. We all accept the need for higher ventilation rates to reduce the risk of transmission; however, tension prevails between working towards greater energy efficiency, achieving net-zero, and meeting ventilation needs.

Most of the buildings where we will live in the coming decades have already been built; in my presentation, I will show how field experiments allow us to understand these buildings. The work we have done and the solutions we have proposed – for example, how to ventilate makeshift hospitals in extremely resource and time limiting situations – are relevant for retrofitting existing buildings in order to create a resilient and sustainable built environment.

Is localised extraction effective at reducing the spread of respiratory droplets?

Cathal Cummins

Heriot-Watt University

O. J. Ajayi (University of Warwick); F. V. Mehendale (University of Edinburgh); R. Gabl (University of Edinburgh); I. M. Viola (University of Edinburgh)

Minisymposium: Modelling the respiratory transmission of Covid-19

The issue surrounding safety and fallow times within dental clinics is an ongoing concern across the globe during the pandemic. In particular, the risk of infection from small droplets from aerosol-generating procedures (AGPs) and respiratory droplets was very much unknown early on in the pandemic. Many surgeries have had to effectively cease their day-to-day operations in order to mitigate potential risks of transmission.

Our understanding of airborne transmission has developed significantly over the course of the pandemic, and it is now recognised that smaller droplets in the air can be just as hazardous as the larger droplets that are typically caught by PPE. Covid-19 guidance from the World Health Organisation was updated only quite recently to reflect the risk of airborne transmission of the virus and, with dental surgeries re-opening, there is an emerging need to ensure the safety of dentists and patients during AGPs.

One potential way to reduce transmission risk in surgeries is to introduce a system to extract contaminated aerosol as close to its source as possible and reduce the volume of aerosol that can spread across a room, therefore, keeping any contamination risks contained to a smaller area. However, the efficacy of such a device for different droplet sizes has not been examined before. In this talk, I will present a simple mathematical model of droplet dispersion and use it to examine the efficacy of localised extraction for a range of droplet sizes.

Modelling and simulation of airborne virus transmission: Present and Future

Dimitris Drikakis

University of Nicosia

Talib Dbouk, University of Lille

Minisymposium: Modelling the respiratory transmission of Covid-19

We developed an innovative numerical frame to investigate airborne virus transmission based on computational multiphysics models. The above includes the accurate modelling and simulation of different multiscale phenomena that involve particles, such as transport, dispersion, breakup, coalescence, filtration and evaporation. Using the above models, we study the advanced physics of virus-contaminated saliva droplets emitted by a human, i.e., from a cough or a sneeze, subject to different conditions of the surrounding environment (temperature, relative humidity and wind speed). We shed light on: i- the social distance in the presence of wind, ii- the efficiency of face masks, iii- the weather effects on airborne virus survival and transmission, iv- the transmission in elevators and confined spaces and v- how computational fluid dynamics can be employed in the pandemic, seasonal forecasting by its coupling with epidemiological models.

A spatially dependent model for rapid prediction of airborne transmission of Covid-19.

Ian Griffiths

University of Oxford

Zechariah Lau (Cardiff University, University of Oxford), Aaron English (University of Manchester) and Katerina Kaouri (Cardiff University)

Minisymposium: Modelling the respiratory transmission of Covid-19

As we begin to learn to live with Covid-19, there is a pressing need to find ways to safely resume economic and social activities while mitigating the viral spread. Probabilistic models for indoor airborne transmission of viruses, such as the Wells Riley model (Riley et al., 1978) and its extensions applied to Covid-19, for example (Buonanno et al., 2020), assume that the concentration of infectious particles in the room is uniform in space. While this gives an estimate for the likelihood of contracting the virus in a given indoor space, it provides no information about how this probability of contraction depends on different locations in the room. In this talk, we present an efficient, holistic model for determining the spatiotemporal risk of infection from Covid-19 in indoor spaces. The airborne infectious particles are emitted by an infected person, advected by airflow, diffused due to turbulence, and removed due to the room ventilation, biological inactivation of the virus and gravitational settling. We model these processes using an advection diffusion reaction equation and determine the concentration of the particles in the room, leveraging the semi-analytic solution to enable fast simulations. The model allows us to quickly determine the time to probable infection and good agreement with CFD models and existing data has been demonstrated. This work has been developed in collaboration with the Welsh Government and paves the way for formulating policy recommendations.

Lifetime of respiratory saliva droplets

Avshalom Offner

The University of Edinburgh

Jacques Vanneste

Minisymposium: Modelling the respiratory transmission of Covid-19

Respiratory transmission by airborne droplets is the leading mechanism by which SARS-CoV-2 spreads. While precautionary measures such as wearing face coverings and maintaining social distancing help reduce this spread, little is known about the airborne lifetime of respiratory droplets, which can remain infectious for well over an hour. In this talk I will present the model we formulated for the dynamics of respiratory saliva droplets, with which we quantified the relative contribution of key factors to the airborne lifetime of virus-carrying droplets. The model is based on Maxey-Riley model a comprehensive momentum balance on suspended particles with which we calculate the spread of respiratory droplets, accounting for their size evolution as they undergo vaporisation via mass and energy balances. The model shows how an increase in relative humidity, which slows the vaporisation rate, leads to larger descent rates that shorten the lifetime of droplets and therefore reduce the risk of transmission. Emulating indoor air turbulence using an Ornstein-Uhlencek process, we numerically calculate probability distributions for the lifetime of droplets, showing how an increase in the air turbulent velocity significantly enhances the range of lifetimes. The distributions strongly deviate from Gaussian statistics, revealing non-negligible probabilities for very long lifetimes, which potentially escalate the risk of transmission.

Micro-particle expiratory ejecta driven by buoyant vortex dynamics

Emiliano Renzi

Loughborough University

Minisymposium: Modelling the respiratory transmission of Covid-19

We investigate the dynamics of the expiratory cloud ejected during human respiratory events. We show that the essential fluid dynamics of the system can be modelled using the theory of buoyant vortex rings with an initial momentum. This allows us to calculate the trajectories of mucosalivary droplets suspended within the cloud, idealised as inert spheres. Our results agree well with available experimental data. The vortex has a significant effect on suspending the droplets in the cloud, increasing the time they remain airborne. This dynamics extends droplet range further than predicted by existing models.

A dissipative Nonlinear Schrödinger model for surface waves propagating in sea ice

Alberto Alberello

University of East Anglia

Emilian Parau (University of East Anglia)

Minisymposium: Nonlinear Surface and Internal Waves

Sea ice attenuates incoming surface gravity waves generated over the open ocean. Here we model propagation of energetic random waves in ice-covered waters with a nonlinear Schrödinger type equation, with an additional dissipative term with a power law dependence on the frequency consistent with current model paradigms and recent field observations. For strong ice-induced dissipation, wave decay is less than exponential due to preferential dissipation of the higher frequency components of the wave spectrum that results in a concurrent significant apparent downshift of the spectral peak. For weak ice-induced dissipation the downshift is less conspicuous, and attenuation is closer to exponential. Dissipation and downshift overcome wave nonlinearity, even for weak ice-induced attenuation, and nonlinear wave statistics at the edge reverts to Gaussianity farther into sea ice.

Internal solitary wave shoaling and the effect of stratification

Magda Carr
Newcastle University

Minisymposium: Nonlinear Surface and Internal Waves

Internal solitary waves (ISWs) are finite amplitude waves of permanent form that travel along density interfaces in stably stratified fluids. They owe their existence to an exact balance between non-linear wave steepening effects and linear wave dispersion. They are common in all stratified flows especially coastal seas, straits, fjords and the atmospheric boundary layer. In the ocean, they are thought to be a source of mixing, and are important in re-suspension of sedimentary materials, and mixing processes in the benthic boundary layer. They are subsequently of interest from both an environmental and offshore engineering point of view.

In this presentation a combined experimental and numerical study will illustrate the effect of stratification form on the shoaling characteristics of internal solitary waves propagating over a smooth, linear topographic slope. It is found that the form of stratification affects the breaking type associated with the shoaling wave. In a thin tanh stratification (homogeneous upper and lower layers separated by a thin pycnocline), good agreement is seen with past studies. Waves over the shallowest slopes undergo fission. Over steeper slopes, the breaking type changes from surging, through collapsing to plunging with increasing wave steepness Aw/Lw for a given topographic slope, where Aw and Lw are incident wave amplitude and wavelength, respectively. In a surface stratification regime (linearly stratified layer overlaying a homogeneous lower layer), the breaking classification differs from the thin tanh stratification. Plunging dynamics are inhibited by the density gradient throughout the upper layer, instead collapsing-type breakers form for the equivalent location in parameter space in the thin tanh stratification. In the broad tanh profile regime (continuous density gradient throughout the water column), plunging dynamics are likewise inhibited and the near-bottom density gradient prevents the collapsing dynamics as well. Instead, all waves either fission or form surging breakers. As wave steepness in the broad tanh stratification increases, the bolus formed by surging exhibits evidence of Kelvin-Helmholtz instabilities on its upper boundary. In both two- and three-dimensional simulations, billow size grows with increasing wave steepness, dynamics not previously observed in the literature.

Theoretical and numerical investigations of extreme waves through oblique soliton interactions

Anna Kalogirou

University of Nottingham

Junho Choi (UNIST, South Korea), Onno Bokhove (University of Leeds)

Minisymposium: Nonlinear Surface and Internal Waves

Extreme water-wave motion is investigated analytically and numerically by considering two-soliton and three-soliton interactions on a horizontal plane. We successfully determine numerically that soliton solutions of the unidirectional Kadomtsev-Petviashvili equation (KPE), with equal far-field individual amplitudes, survive reasonably well in the bidirectional and higher-order Benney-Luke equations (BLE). A well-known exact two-soliton solution of the KPE on the infinite horizontal plane is used to seed the BLE at an initial time, and we confirm that the KPE-fourfold amplification approximately persists. More interestingly, a known three-soliton solution of the KPE is analysed further to assess its eight- or ninefold amplification, the latter which only exists in a special and difficult to attain limit. This solution leads to an extreme splash at one point in space and time. Subsequently, we seed the BLE with this three-soliton solution at a suitable initial time to establish the maximum amplification: it is approximately 7.8 for a KPE amplification of 8.4. In our simulations, the computational domain and solutions are truncated approximately to a fully periodic or half-periodic channel geometry of sufficient size, essentially leading to cnoidal-wave solutions. Moreover, special geometric (finite-element) variational integrators in space and time have been used so that artificial, numerical damping, in particular of wave amplitude, is zero.

Transition from elongating to squeezed interfacial ring waves on a current

Karima Khusnutdinova

Department of Mathematical Sciences, Loughborough University

Curtis Hooper (Loughborough University), Roger Grimshaw (University College London)

Minisymposium: Nonlinear Surface and Internal Waves

The usual surface ring waves propagating over a parallel current have elongated wavefronts. It transpired that in some cases interfacial ring waves propagating over the same current could be squeezed. The only example to date described long interfacial waves in a two-layer fluid over a piecewise-constant current [1]. We now show that there is a transition from the regime of elongating to squeezed wavefronts for the long interfacial ring waves in a two-layer fluid over a large family of power-law upper-layer currents tending to a piecewise-constant current [2]. For different powers, the currents could be used to model wind-generated currents, river inflows and exchange flows in straits. The 2D long-wave dispersion relation is given in terms of the hypergeometric functions. We introduce and use global (distance) and local (curvature) measures for the deformation of wavefronts.

[1] K.R. Khusnutdinova, X. Zhang, Long ring waves in a stratified fluid over a shear flow, J. Fluid Mech. (2016), vol. 794, 17-44. [2] C. Hooper, K. Khusnutdinova, R. Grimshaw, Wavefronts and modal structure of long surface and internal waves on a parallel shear current, J. Fluid Mech. (2021), vol. 927, A37.

The Crawford-Saffman-Yuen equation and evolution of inhomogeneous sea-states

Raphael Stuhlmeier

University of Plymouth

David Andrade (Plymouth), Michael Stiassnie (Technion)

Minisymposium: Nonlinear Surface and Internal Waves

The nonlinear interaction of surface water waves is a key ingredient in modern wave forecasting. For statistically homogeneous sea states, the four-wave kinetic equation developed by Hasselmann captures the resulting energy exchange over long time-scales. However, faster spectral changes are also possible with departures from homogeneity. I will review recent advances in understanding the stability and evolution of broad-banded inhomogeneous sea-states using an equation originally developed by Crawford, Saffman and Yuen.

A theory for steady parasitic capillary ripples on steep gravity waves

Phil Trinh

University of Bath

Josh Shelton (Bath) and Paul Milewski (Bath)

Minisymposium: Nonlinear Surface and Internal Waves

It is known, both from observation and intuition, that under the action of gravity and surface tension, ripples of small wavelength often form near the crest of a steep propagating water wave. Surprisingly, analytical theory of these 'parasitic' ripples remains elusive. In the talk, I will describe some of the early works of Longuet-Higgins in proposing an asymptotic theory for such ripples. I will report on our recent numerics that have revealed the complex structure arising in the small surface tension limit, and I will also present the key ideas of how exponential asymptotics can describe the emergence of such parasitic ripples. This forms joint work with Josh Shelton (Bath) and Paul Milewski (Bath).

Nonlinear triad interactions of acoustic-gravity waves

Usama Kadri
Cardiff University

Minisymposium: Nonlinear Waves and Jets

Acoustic (compression) waves and free-surface (gravity) waves are virtually decoupled for two main reasons. Firstly, the speed of sound in water far exceeds the maximum phase speed of gravity waves. Secondly, the mode shape with depth is oscillatory for acoustic modes, and exponentially decaying for gravity waves. Nevertheless, it has been argued theoretically that these two types of wave motion could exchange energy via resonant triad nonlinear interactions [1-5]. There are two cases of interest this review talk focuses on: (I) two gravity waves interacting with an acoustic mode of a comparable frequency (almost double) [1-3]; and (II) two acoustic modes interact with a gravity wave of a comparable lengthscale [4-5]. In the first case, the theory suggests that for a perfectly tuned triad almost all energy initially stored in the gravity waves can transfer into the generated acoustic mode, whereas for wavepackets a maximum of 40% energy transfer can be obtained [2]. This has implications at the ocean scale where interacting surface gravity waves can generate microseism (faint earth tremor) deep at the ocean floor [6-7]. Not less interestingly is the particular solution where two gravity waves of identical frequency generate a standing acoustic mode [8]. Such setting might explain a physical phenomenon known as time reversal [9-10]. The same solution might explain the evolution of Faraday waves [8,11] that find various applications in physics. In the second case, the interaction of two acoustic modes with one gravity wave has implications on underwater communication [4], wave energy harnessing, or more ambitiously tsunami mitigation [5].

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Heat transfer in the seabed laminar boundary layer

Simone Michele

University of Plymouth

Raphael Stuhlmeier and Alistair Borthwick. University of Plymouth.

Minisymposium: Nonlinear Waves and Jets

We present a theoretical model of the temperature distribution in the boundary layer region close to the seabed. Using a perturbation expansion, multiple scales and similarity variables, we show how free-surface waves enhance heat transfer between seawater and a seabed with a solid, horizontal, smooth surface. Maximum heat exchange occurs at a fixed frequency depending on ocean depth, and does not increase monotonically with the length and phase speed of propagating free-surface waves. Close agreement is found between predictions by the analytical model and a finite-difference scheme. It is found that free-surface waves can substantially affect the spatial evolution of temperature in the seabed boundary layer. This suggests a need to extend existing models that neglect the effects of a wave field, especially in view of practical applications in engineering and oceanography.

Deformation and dewetting of liquid films under gas jets

Juliet Chinasa Ojiako

Loughborough University

Radu Cimpeanu (University of Warwick) Hemaka Bandulasena, Roger Smith, Dmitri Tseluiko (Loughborough University)

Minisymposium: Nonlinear Waves and Jets

We study the deformation and dewetting of a liquid film in a cylindrical beaker under the influence of an impinging gas jet. To obtain initial insight into relevant regimes and timescales of the system, we first derive a reduced-order model (a thin-film equation) based on the long-wave assumption and on appropriate decoupling the gas problem from that for the liquid [1-3] and taking into account a disjoining pressure [4]. We also perform direct numerical simulations (DNS) of the full governing equations using two different approaches, the Computational Fluid Dynamics (CFD) package in COMSOL and the volume-of-fluid Gerris package. The DNS are used to validate the results for the thin-film equation and also to investigate the regimes that are beyond the range of validity of this equation. We additionally compare the computational results with experiments and find good agreement.

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Wave Dynamics in the Neighbourhood of the Benjamin-Feir Instability

Daniel Ratliff

Northumbria University

Tom Bridges, University of Surrey; Olga Tritchenko, University of Western Ontario

Minisymposium: Nonlinear Waves and Jets

The dynamics of dispersive nonlinear waves remains a problem that attracts significant interest, in part for their interesting stability properties. Arguably the most famous case is the Benjamin-Feir (BF) instability, where uniform wavetrains undergo a transition of stability due to a nonlinear frequency correction term $\omega_2(k)$, which depends on the wavenumber k. This transition occurs precisely when $\omega_0(k)''\omega_2 = 0$, where $\omega_0(k)$ is the linear dispersion relation and primes denotes differentiation. There are several emergent behaviours in the neighbourhood of this transition, such as an increase in the wave's wavelength (frequency downshifting) or resonant wave bursting, which have been observed but elude mathematical insight as to why they might occur.

To best understand these phenomena, we revisit the seminal work of Whitham by augmenting his modulation theory with ideas from phase dynamics. This ultimately reveals that each of the possible transitions (either $\omega_0'' = 0$ or $\omega_2 = 0$) admits a different set of nonlinear dispersive dynamics governing the wave quantities whose solutions can be used to understand the wave behaviours near the BF threshold. Moreover, this work illustrates the role of mean flow is significant and is central to the emergence of permanent frequency downshifting and localised wave bursts one observes. We use this reasoning to explain, at least qualitatively, the experimental observations from wave-tank experiments in water waves and fluid conduits.

Nonlinear dispersive waves generated by moving seabed deformation

Emiliano Renzi

Loughborough University

S. Michele, A.C. Raby, A.G.L. Borthwick

Minisymposium: Nonlinear Waves and Jets

We present a weakly nonlinear theory for the evolution of fully dispersive transient waves generated by moving seabed deformation. Using a perturbation expansion technique, we show that higher-order components affect mostly the leading wave and the region close to the deforming seabed. In particular, the leading wave in the nonlinear regime has higher crests and deeper troughs than the known linear solution, while the trough that propagates together with the moving seabed exhibits a pulsating behaviour. We compare our solution with existing models based on the Boussinesq approximation for weakly dispersive waves, showing that the latter fails in describing the dispersive behaviour of the trailing wave system. We then consider fully nonlinear aspects using a Lagrangian mesh-free model. We show that as the

deformation speed approaches the critical value, a large leading elevation wave is generated, travelling faster than predicted by linear theory. This crest is followed by a trail of dispersive short and steep waves, of which we investigate the breaking dynamics. The model is validated with respect to available experimental and analytical data.

Entropic Variational Schemes for Non-Gradient Systems.

Daniel Adams
University of Edinburgh
Gonalo dos Reis (University of Edinburgh). Hong Duong (University of Birmingham).

Minisymposium: Nonreversible processes: analysis and computations

Over the past twenty years it has become popular to identify the Wasserstein space with a Riemannian structure. Many well-known and widely studied PDE have been shown to be a Wasserstein gradient flow (WFG) of an associated energy functional. Famously, the Heat Equation is a WGF of the (negative) Boltzman entropy, and the Porous Medium Equation is a WGF of its internal energy. One way of identifying this structure is through an implicit Euler scheme of the WGF, known as the 'JKO scheme', giving credit to the seminal work of Richard Jordan, David Kinderlehrer, and Felix Otto, who were the first to prove the convergence of such a scheme. Many PDE are not gradient flows, but still possess a Lyapunov structure. We will present some variational schemes for these these systems akin to the 'JKO scheme'. The schemes are regularized allowing for fast computation of the Wasserstein distance via Sinkhorns Algorithm.

Piecewise Deterministic Monte Carlo in Infinite Dimensions

Joris Bierkens
Delft University of Technology
Paul Dobson (Edinburgh)

Minisymposium: Nonreversible processes: analysis and computations

In Bayesian inverse problems one is interested in performing computations with respect to an infinite dimensional probability distribution. A modern computational approach consists of approximating this infinite dimensional probability distribution by running a truncated version of a genuine infinite dimensional Markov chain. If a well-posed infinite dimensional chain exists, then the truncated, finite-dimensional approximation may be expected to have desirable scaling properties with respect to dimension.

In this talk we present some explorations of this topic in conjunction with the recent advance of Piecewise Deterministic Monte Carlo methods such as the Bouncy Particle Sampler and the Zig-Zag Sampler and more recently the Boomerang Sampler. In particular we provide a general construction of Piecewise Deterministic Markov Processes with unbounded event rates in infinite dimensional spaces, we study the wellposedness of infinite dimensional versons of the the Zig-Zag Sampler, Bouncy Particle Sampler, and the Boomerang Sampler, and for the Boomerang Sampler we provide exponential ergodicity result by means of hypocoercivity techniques.

Geometric integrators for optimization

Guilherme Franca
University of California, Berkeley, USA

Minisymposium: Nonreversible processes: analysis and computations

Symplectic integrators are often the preferred integration scheme for simulating conservative Hamiltonian systems with important applications in statistical mechanics, Monte Carlo methods, and numerical simulations of gauge field theories. Their success is due to the fact that, besides exactly preserving the symplectic structure, they preserve the Hamiltonian within a bounded error. However, this result depends crucially on the fact that the Hamiltonian is a constant of motion. We will show how this result can be extended into dissipative settings where such conservation law no longer applies. We will also extend this perspective to constrained cases on arbitrary manifolds. In particular, this approach enables one to construct a large class (accelerated) optimization methods with interesting applications in machine learning.

Design and Implementation of PDMP Monte Carlo Methods

Sam Power
University of Bristol, School of Mathematics

Minisymposium: Nonreversible processes: analysis and computations

The application of Piecewise-Deterministic Markov Processes (PDMPs) to Monte Carlo simulation has garnered some attention in recent years, due in part to to their appealing non-reversible character. In this talk, I will discuss some aspects of how to design these processes in order to produce the desired equilibrium behaviour, as well as describing a simple-but-nonstandard practical implementation which enables their application to a relatively generic class of problems.

Variational formulations beyond gradient flows

Michiel Renger
WIAS Berlin
Robert I.A. Patterson (WIAS Berlin), Upanshu Sharma (FU Berlin)

Minisymposium: Nonreversible processes: analysis and computations

It is well known that large deviations of reversible processes can be related to entropic gradient flows; this proves a physically meaningful variational structure that can also be useful for computations. In this work we look for a more general variational structure for nonreversible processes. We use modern techniques from macroscopic fluctuation theory to uniquely decompose the large deviations into a gradient flow and a dynamics that is in some sense the exact "opposite" of a gradient flow. It turns out that this dynamics is often a Hamiltonian system.

Imbedding Deep Neural Networks

Andrew Corbett
University of Exeter

Minisymposium: Reservoir Computing and Dynamical Systems

Continuous depth neural networks, such as Neural ODEs, have refashioned the understanding of residual neural networks in terms of non-linear vector-valued optimal control problems. The common solution is to use the adjoint sensitivity method to replicate a forward-backward pass optimisation problem. We propose a new approach which explicates the network's 'depth' as a fundamental variable, thus reducing the problem to a system of forward-facing initial value problems. This new method is based on the principle of 'Invariant Imbedding' for which we prove a general solution, applicable to all non-linear, vector-valued optimal control problems with both running and terminal loss. Our new architectures provide a tangible tool for inspecting the theoretical–and to a great extent unexplained–properties of network depth. They also constitute a resource of discrete implementations of Neural ODEs comparable to classes of imbedded residual neural networks.

An invitation to Echo State Networks

Jonathan Dawes

University of Bath

Allen Hart (Bath), James Hook (Jump Trading LLC)

Minisymposium: Reservoir Computing and Dynamical Systems

This presentation will provide a general introduction, suitable for non-specialists, to Echo State Networks (ESNs) which are a computationally simple, practically useful, and mathematically attractive example of reservoir computing and which will be a recurrent reference point throughout the minisymposium.

Specifically I will consider ESNs trained on noise-free input sequences of observations from a deterministic dynamical system and explore to what extent we can prove that the ESN dynamics resembles the dynamics of the original dynamical system. We prove three fundamental and reassuring aspects of ESN construction and behaviour that between them help to explain the success of ESNs in reliably capturing dynamical behaviour.

Reference: A.G. Hart et al, *Neural Networks* **128**, 234-247 (2020).

Modelling transitions in epileptic seizure dynamics with a multifunctional reservoir computer

Andrew Flynn

University College Cork

Cian McCafferty (University College Cork), Vincenzo Crunelli (Cardiff University), Franois David (Paris Descartes University), Vassilios A. Tsachouridis (Collins Aerospace), and Andreas Amann (University College Cork)

Minisymposium: Reservoir Computing and Dynamical Systems

In this talk we explore how to reconstruct dynamical transitions present in the epileptic brain using the reservoir computing approach to machine learning. Using experimental neural voltage data obtained from epileptic rodent brains, we train a reservoir computer (RC) to provide a coexistence of the seizure and non-seizure dynamical regimes. This results in a multifunctional RC which can simultaneously reconstruct the long term behaviour of multiple attractors. By destabilising this multifunctional RC we then enable it to display chaotic itinerancy as its state wanders between the seizure and non-seizure modes of operation, thereby exhibiting similar dynamics to the epileptic brain.

Learning with Reservoir Computing: Geometric perspective and open problems

Lyudmila Grigoryeva
University of Warwick (Department of Statistics)

Minisymposium: Reservoir Computing and Dynamical Systems

In this presentation, we will discuss families of reservoir systems, their main functional and statistical properties. Reservoir computing is understood in the literature as the possibility of approximating input/output systems and dynamical systems with random-weights recurrent neural systems and a trained linear readout layer. We will talk about possible explanations of the excellent performance of reservoir computing in the learning of dynamic processes both in the deterministic and stochastic settings. In particular, we will take a geometric perspective and provide a connection to discrete-time signatures. We will conclude with some open problems arising when attempting to reconstruct deterministic dynamical systems out of noisy observations as well as when learning stochastic processes or their conditional moments.

This presentation is mostly based on a series of joint works with J.-P. Ortega as well as recent contributions together with C. Cuchiero, L. Gonon, A. Hart, J.-P. Ortega, and J. Teichmann.

Learning strange attractors with reservoir systems

Allen G Hart
University of Bath
Juan-Pablo Ortega, NTU Singapore, Lyudmila Grigoryeva, Warwick UK

Minisymposium: Reservoir Computing and Dynamical Systems

In this talk we discuss how the celebrated Embedding Theorem of Takens is a particular case of a much more general statement according to which, randomly generated linear state-space representations of generic observations of an invertible dynamical system carry in their wake an embedding of the phase space dynamics into the chosen Euclidean state space. This embedding coincides with a natural generalized synchronization that arises in this setup and that yields a topological conjugacy between the state-space dynamics driven by the generic observations of the dynamical system and the dynamical system itself. This result provides additional tools for the representation, learning, and analysis of chaotic attractors and sheds additional light on the reservoir computing phenomenon that appears in the context of recurrent neural networks.

A Machine Learning Perspective on Driven Dynamical Systems

Peter Tino

University of Birmingham

Minisymposium: Reservoir Computing and Dynamical Systems

This presentation will outline a possible framework for studying parametrised input-driven dynamical systems, such as Echo State Networks. Rather than generalising concepts from theory of autonomous dynamical systems, we will be inspired by the theory of feature spaces and kernel machines from the field of Machine Learning.

In particular, I will first present ideas of kernel machines and then apply them to analysing input-driven dynamical systems that represent the driving sequences through their state spaces. This viewpoint will enable us to understand properties of such systems that have been empirically observed but so far not theoretically understood. I will also present open problems that such a framework naturally poses.

Reference: P. Tiňo, *Journal of Machine Learning Research* 21(**44**), 1-42 (2020).

Two-dimensional nematics and their applications

Apala Majumdar

University of Strathclyde

Yucen Han, James Dalby, Joseph Harris, Lei Zhang

Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

Nematic liquid crystals are classical examples of partially ordered materials that combine fluidity with long-range orientational order. We model nematics in a thin-film scenario or approximately two-dimensional settings i.e. nematics on surfaces, within a reduced Landau-de Gennes modelling framework. We study the interplay between the material properties and surface properties for the corresponding solution landscapes i.e. the multiplicity and structural details of stable equilibria, and transition pathways between distinct equilibria. We also study the crucial role of nematic defects in tailoring solution landscapes; these defects manifest as localised regions of vanishing nematic order on the surfaces and could act as distinguished or binding sites in applications. We conclude with some discussions on how to construct three-dimensional solution landscapes from these reduced studies, and their potential applications for opto-electronic devices and materials technologies.

Smectic Layering: A Complex Tensor Representation

Jack Paget
Loughborough University
Jack Paget,[1] Marco G. Mazza,[1,2] Andrew J. Archer,[1] and Tyler N. Shendruk[3].
[1] *Loughborough University*
[2] *MPI for Dynamics and Self-Organization*
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Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

Smectic materials represent a distinct state of matter between solids and fluids, characterised by the coexistence of partial ordering and self-assembly into layers. While being excellent systems for exploring topology and defect interactions, these anisotropic properties make them notoriously difficult to model, particularly in confinement.

We use a novel complex tensor order parameter to describe the local degree of lamellar ordering, layer displacement and orientation, and demonstrate its capability in describing both dislocations and disclinations, as well as arrested configurations and colloid-induced local ordering. This theory accounts for both parallel and perpendicular elastic contributions, reduces to previous employed models of simple smectics and can be easily coupled to existing nematic descriptions. While being versatile, it considerably simplifies numerics, facilitating new studies of smectic phases and their topological defects under large deformations in non-trivial geometries.

Theories of smectic A liquid crystals: a critical discussion

Timothy J. Sluckin
School of Mathematics, University of Southampton SO17 1SY

Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

The smectic liquid crystal phases consist usually of symmetric layers. In an ideal case these layers are arranged, bookshelf-like, without any layer defects, and subject only to small fluctuations around the bookshelf structure. However, observation of this ideal structure requires a scattering experiment. The original microscopic observations under crossed polars appeared to demonstrate the existence of focal conic lines. In 1922, Georges Friedel realised that these focal conic lines were macroscopic signatures of a defected layered structure. In many smectic samples (for simplicity consider the smectic A phase in which the director is normal to the layers) defect lines, both dislocations and disclinations, abound, and the question of a consistent mesoscopic description, including simultaneously the nematic-smectic phase transition, smectic hydrodynamics and layer defects, is not clear.

The simplest hydrodynamic models involve level sets, while de Gennes introduced a model in which the smectic order parameter $\Psi(\mathbf{r}) = \rho e^{i\phi}$, where ρ represents the

maximal density fluctuation around the mean, and ϕ is the phase of this density fluctuation, pointing out the analogy with type 2-superconductors. This analogy has been fruitful, but it is now realised that it is incomplete. It fails to take into account the symmetry between the Ψ and Ψ^* descriptions. The most serious implication is that the de Gennes theory is unable to describe half-integer disclinations, and the Peierls-Nabarro barrier for dislocation slip vanishes.

About a decade ago, in collaboration with Pevnyi and Selinger, I introduced a simple density functional caricature of the smectic phase which no longer possesses these difficulties, but only at the cost of losing the advantages of the phenomenological de Gennes approach. Other workers have tried, in various different ways, to modify the de Gennes model in such a way as to avoid the difficulties while maintaining its many convenient facets. In this talk, I shall discuss critically theories of the smectic phase with a view to making progress to a more complete phenomenolgical picture.

Key Words: Smectic Liquid Crystals; Defects; Order Parameter; Topology; Hydrodynamics

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Smectic A liquid crystals in non-uniform domains: Modelling the impact of imperfect boundaries

Alan J. Walker

University of the West of Scotland

Ayad S. al Sallo, University of South Wales, Graeme P. Boswell, University of South Wales

Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

We consider the construction of equilibrium configurations for smectic A liquid crystals subjected to nonuniform physical boundary conditions, with two-dimensional dependence on the director and layer normal, and a nonlinear layer function.

Euler-Lagrange equations are constructed that describe key properties of liquid crystals confined between two boundaries exhibiting spatial imperfections. Domain sizes are considered representing those currently used in applications while predictions in smaller domains at the limit of current technologies are also made.

We illustrate that the curvature along a boundary impacts on the liquid crystal's structure distant from the boundary feature, causing issues for some technologies but potentially opening doors for others.

New patterns of twist-bend liquid crystal phase behaviour

Rebecca Walker
University of Aberdeen
Ahlam Alshammari, Ewan Cruickshank, John MD Storey and Corrie T Imrie (University of Aberdeen); Damian Pociecha, Ewa Gorecka (University of Warsaw)

Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

Over a decade since they were first theorized,[1,2] heliconical liquid crystal phases formed by achiral, bent-shaped molecules constitute the newest class of liquid crystal phases and have attracted considerable global research interest. The twist-bend nematic phase, NTB, is an intriguing and unique example of spontaneous mirror symmetry breaking in a fluidic state; a locally chiral phase formed from achiral molecules. In the NTB phase, the director forms a helix and is tilted with respect to the helical axis; the spontaneous formation of chirality ensures that equal numbers of left- and right-handed degenerate helices are formed.[3] More recently, heliconical twist-bend smectic C (SmCTB) phases have also been discovered for liquid crystal dimers[4,5] and in bent-core mesogens,[6] and it appears that a range of variants of this phase, similar to the SmC* subphases observed for chiral molecules, are possible.

Here we report the synthesis and extensive characterisation of several new homologous series of liquid crystals, showing rich liquid crystal polymorphism including twist-bend nematic and smectic phases. Despite the molecules themselves being achiral, fascinating phenomena observed for these series include the transition between a phase with a single short helix and phase with a double helix, structural chirality at different length-scales and the exhibition of a photonic bandgap for visible light.

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A Q-tensor model of smectic-A liquid crystals and its numerical analysis

Jingmin Xia

National University of Defense Techonology

Minisymposium: Smectic Fluids: Reduced Dimensionality/Increased Complexity

In this talk, we propose a new continuum model, solving for a real-valued smectic order parameter for the density variation and a tensor-valued nematic order parameter for the director orientation. This expands on an idea mentioned by Ball & Bedford. The model is challenging to discretise due to the high regularity of the density variation; to address this, a continuous interior penalty discretisation is employed. Numerical analysis and experiments are performed to confirm the effectiveness of the proposed model and discretisation. The model numerically captures important defect structures in focal conic domains and oily streaks. This work has been published in PRL.

Analytical continuation of two-dimensional wave fields

Raphael Assier

The University of Manchester

Andrey Shanin, Moscow State University

Minisymposium: Wave Problems in Complex Continua

In this talk, we will consider a wide range of two-dimensional diffraction problems and ask ourselves the following question: what happens to the solution of these diffraction problems when the space variables are complexified? We will devise a systematic way of analytically continuing these physical solutions as functions of two complex variables (and explain what we mean by this!). The singularities of the resulting (multi-valued) analytical continuation will be studied and we will show that it is possible to describe all the infinitely many possible values of this function in terms of a finite set of basis functions. Each basis function will be expressed explicitly as a Green's integral over a double-eight (or Pochhammer) contour. Finally, we will show how this finite basis property can be used to obtain precious information on the actual physical solution of the diffraction problem at hand.

This is a joint work with Dr Andrey Shanin from Moscow State University and linked to the following article: R.C. Assier and A.V. Shanin, Analytical continuation of two-dimensional wave fields, Proc. Roy. Soc. A, 477:2020081, 2021 (open access)

Ray-tracing the Ulam way

David Chappell

Nottingham Trent University

Julia Slipantschuk (University of Warwick), Martin Richter, Gregor Tanner (University of Nottingham), Wolfram Just, Oscar Bandtlow (Queen Mary University of London)

Minisymposium: Wave Problems in Complex Continua

Ray-tracing is a well established approach for modelling wave propagation at high frequencies, in which the ray trajectories are defined by a Hamiltonian system of ODEs. An approximation of the wave amplitude is then derived from estimating the density of rays in the neighbourhood of a given evaluation point. An alternative approach is to formulate the ray-tracing model directly in terms of the ray density in phase-space using the Liouville equation. The solutions may then be expressed in integral form using the Frobenius-Perron operator, which is a transfer operator transporting the ray density along the trajectories. The classical approach for discretising such operators dates back to 1960 and the work of Stanislaw Ulam. The convergence of the Ulam method has been established in some cases, typically requiring the trajectory flow map of the dynamical system to be expanding. In this talk we discuss recent work investigating the convergence of the Ulam method for ray tracing in triangular billiards, where the dynamics are parabolic and the flow map contains jump discontinuities.

Ultrasonic measurement of stress without material constants

Artur Gower

University of Sheffield

Michel Destrade - NUI Galway, Guoyang Li - Harvard Medical School and Wellman Center for Photomedicine

Minisymposium: Wave Problems in Complex Continua

Elastic and acoustic waves are in many ways ideal to probe materials: they travel with ease in most solids, are easy to generate, and are non-destructive (in contrast to say X-rays or drilling holes). It has long been known that we can estimate the stress from the time it takes for a shear wave (polarised in the stress plane) to travel, because the higher the stress, the faster the shear wave will travel. However, this knowledge has not led to robust measurement techniques because the wave speed also depends on other factors, such as the material's elastic constants. For example, the higher the Young's modulus the faster the waves travel, irrespective of the stress.

In this talk, I will show how we can use universal relationships between stress and wave speeds to design measurements which do not need this prior knowledge of the materials elastic constants. Although I will focus on measuring stress, a similar procedure could be used to design other measurements from anisotropic materials based on universal relationships.

Surface waves in nonlocally elastic solids

Ludmila Prikazchikova

School of Computer Science and Mathematics, Keele University

Julius Kaplunov and Danila Prikazchikov, School of Computer Science and Mathematics, Keele University

Minisymposium: Wave Problems in Complex Continua

Integral and differential formulations in nonlocal elasticity are subject to comparative analysis, resulting in advanced differential model, taking into account the boundary layers localized near free surface. To this end, extra boundary conditions have to be imposed on stresses along the planes orthogonal to the surface which do not appear in the traditional boundary conditions. It is demonstrated that a shear surface wave appears due to the effect of the boundary layer. A nonlocal correction to the classical Rayleigh wave speed is also determined. In addition, it is proved that the previous solutions for nonlocal Rayleigh type waves are erroneous, i.e. they do not satisfy the original equations of motion.

Spectral properties of the chiral orthogonal, unitary, and symplectic ensembles - A microwave realization

Martin Richter

University of Nottingham

Aimaiti Rehemanjiang, Hans-Jrgen Stckmann, Universitt Marburg, Germany and Ulrich Kuhl, Universit Cte d'Azur, France

Minisymposium: Wave Problems in Complex Continua

We will address wave aspects of certain complex, fully chaotic systems, namely such with a chiral symmetry. The presentation will start with a very introductory overview of Random Matrix Theory, RMT, and its link to physical systems and their quantum spectra. In this realm, RMT has proven very successful in the understanding of the spectra of chaotic systems. Depending on symmetry with respect to time reversal and the presence or absence of a spin 1/2 there are three ensembles, the Gaussian orthogonal (GOE), Gaussian unitary (GUE), and Gaussian symplectic (GSE) one. With a further particle-antiparticle symmetry the chiral variants of these ensembles, the chiral orthogonal, unitary, and symplectic ensembles (the BDI, AIII, and CII in Cartan's notation) appear. A microwave study of the chiral ensembles is presented using a linear chain of evanescently coupled dielectric cylindrical resonators [1]. In all cases the predicted repulsion behaviour between positive and negative eigenvalues for energies close to zero could be verified.

[1] https://doi.org/10.1103/PhysRevLett.124.116801, Rehemanjiang et.al, PRL 124, 2020

Absorption characteristics of large acoustic metasurfaces

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Minisymposium: Wave Problems in Complex Continua

Metasurfaces formed of arrays of subwavelength resonators are often tuned to 'critically couple' with incident radiation, so that at resonance dissipation and radiation damping are balanced and as a consequence absorption is maximised. Such design criteria are typically derived assuming an infinite metasurface, whereas the absorption characteristics of finite metasurfaces, even very large ones, can be markedly different. This is owing to the excitation of surface waves, intrinsic to resonant metasurfaces, and meta-resonances, namely collective resonances where surface waves form standing-wave patterns over the finite metasurface domain. We illustrate this matter by studying a reduced model of a Helmholtz-type acoustic metasurface formed of cavity-neck resonators embedded into a rigid substrate, with geometric and dissipation effects included from first principles (R. Brando and O. Schnitzer, Wave Motion, 97 102583, 2020).

An enhanced dipole resonance for elastodynamic metamaterials

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Minisymposium: Wave Problems in Complex Continua

In the framework of metamaterials, which take advantage of a microstructure in order to control the propagation of waves at a macroscopic scale, resonances are of great interest since they allow to reach a subwavelength response. In elasticity, a dipole resonance was first studied in the work of Liu et al. [1] in which a rigid core inclusion is placed in a softer layer of silicone rubber itself placed in a hard epoxy matrix.

The concept of metacluster introduced in Packo et al. [2] takes advantage of a collection of scatterers in a plate in order to tune the far-field flexural wave response due to some incident field. In Cotterill et al. [3], a metacluster of voids leading to a monopole resonance, i.e. voids in an elastic matrix which has a bulk modulus much greater that its shear modulus, is studied and it is shown that the configuration of circular cylindrical voids can have a significant effect on the resonant frequency and the far-field response. In particular it is shown that a collection of voids leads to a much lower resonance than a single void of the same cross-sectional area.

In the present work, we extend the notion of a metacluster to the case of coated cylinders of circular cross-section in a similar vein to Liu et al [1], which consequently give rise to a dipole resonance. More precisely, we study the manner by which the resonance arising from this configuration is affected when two or more such scatterers are in close proximity. We show that reducing the distance between two such scatterers enhances the dipole resonance significantly. Therefore, the scattering amplitude and the directionality can be tailored and tuned, exploiting the geometry of the configuration. Such metaclusters could then be used in the design of elastodynamic metamaterials in order to control both wave propagation and effective dynamic material properties.

[1] Z. Liu, X. Zhang, Y. Mao, Y.Y. Zhu, Z. Yang, C-T. Chan, and P. Sheng. Locally resonant sonic materials. Science, 289(5485):1734-1736, 2000. [2] P. Packo, A.N. Norris, and D. Torrent. Metaclusters for the full control of mechanical waves. Physical Review Applied, 15(1):014051, 2021. [3] P. A. Cotterill, D. Nigro, and W. J. Parnell. Enabling the control of elastic waves with deeply sub-wavelength giant monopole metacluster resonators, submitted to Proceedings of the Royal Society A.

Poster abstracts

Measuring Bipartivity

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Philip Knight

Community detection has been an active area of research in the last fifteen years and has led to a number of very effective algorithms for real world applications. A related topic is the identification of anti-communities, which arise when vertices have most of their connections outside the group have very few (or no) connections inside the same group. In the case where there are no internal connections, the underlying networks are bipartite (or two mode). Thus we might expect to be able to find anti-communities in networks which are close to bipartite. Since bipartivity is a binary condition, closeness to bipartivity is not uniquely define. We give a thorough review of equivalent characterisations of bipartivity and show that many of them lead to (piecewise-)continuous measures: some new and some well-known. But we show that the different characterisations can lead to profoundly different conclusions about the level of bipartivity within a network. For example, we show that is possible to generate a network that is arbitrarily close to being bipartite by one measure while being arbitrarily far by another. We investigate what these means in applications (for example, a difference in two popular measures can indicate a core-periphery structure), we describe how the measures perform on real-world networks which are known to be approximately two-mode and we consider the implications for algorithms used to find anti-communities.

Keywords: Complex network-Graph theory-Matrix algebra

Simulation of crystallisation dynamics of growth dominated phase-change material using the Master rate equation

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Chalcogenide-based phase-change materials are technologically important in non-volatile memory applications such as rewritable DVDs and blu-ray disks, phase-change random access memories (PCRAM) [1], and photonic memories and processors [2]. Subject to specific annealing conditions applied through Joule heating or optical absorption, phase-change materials switch from the disordered amorphous phase to the ordered crystalline phase and vice versa. This switching process is accompanied by changes in the electrical and optical properties of the material or heated region with sufficient contrast to provide the important threshold and memory functions. The kinetic transition process from the amorphous to crystalline phase, or crystallisation, governs the rate of switching and critical temperatures in the material. Thus, understanding of the crystallisation process is critical for controlling the speed of data storage/erasure and data retention in practicable memory devices. Crystallisation normally proceeds through nucleation of critical nuclei followed by their growth, and both of these processes determine the crystallisation time. In a certain class of phase-change materials, crystallisation proceeds mainly through growth at elevated temperatures and hence are called growth dominated material [3]. This leads to benefit not only in increasing the crystallisation rate but also increased phase stability and improved data retention. The aim of this work is to model and simulate numerically the crystallisation process in growth dominated phase-change material using the physically realistic Master rate equation method, to study the crystallisation speed and temperature in these materials under different annealing conditions. The Master rate equation method considers both the attachment and detachment of monomers during crystallisation, and hence naturally traces nucleation and growth of crystallites with temperature history to calculate the distribution of cluster sizes at practical computation times [4]. In particular, we include in the model the fragile-to-strong transition in viscosity with temperature observed experimentally [5] to realistically model the kinetics of crystallisation in growth dominated material. The calculated transient cluster size distributions will be used to study the rate of crystalline fraction transformed and crystallisation temperatures to understand the phase transition mechanism in growth dominated material and explain experimental observations.

[1] Raoux et al., Chem. Rev. 110, 240-267 (2010). [2] Rios et al., Sci. Adv. 5, 1-9 (2019). [3] L. van Pieterson, in “Phase-change materials: science and applications”, Editors: Raoux and Wuttig, Chap. 5, Springer, New York (2009). [4] Aladool et al., J. Appl. Phys. 121, 224504 (2017). [5] Orava et al., Adv. Funct. Mater. 25, 4851-4858 (2015).

Keywords: Growth dominated phase-change materials, the Master rate equation, modelling and simulation, crystallisation process

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Nonlinear waves in Mass-in-Mass FPUT chains

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In this poster, we numerically simulate a chain of particles connected by nonlinear springs, with each particle also connected to an internal nonlinear oscillator. This system is known as a mass-in-mass Fermi-Pasta-Ulam-Tsingou (FPUT) lattice. The system’s linear frequency spectrum is composed of two branches - an ‘optical’ branch of higher frequency modes, and a lower-frequency ‘acoustic’ branch. In the gap between these, and above the optical branch, nonlinear modes are postulated to exist. We consider the case where all interactions have nonlinear components. An asymptotic reduction to the Nonlinear Schrdinger (NLS) equation recovers approximate solitary waves. Our findings show that the system supports stable and unstable stationary breather and breather-kink solutions, as well as an unstable, but long-lived moving breather and breather-kink solutions.

Keywords: nonlinear wave, breather.

The Impact of Episodic Plastic Pollution on Predator-Prey Interactions

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Pre COVID19, plastic pollution was on a par with climate change as the most pressing environmental concern facing society in this millennium. Plastic disrupts the life cycles of various species - both terrestrial and marine. Plastic may directly kill species, e.g. by poisoning, or indirectly, e.g. through disruption of food sources. Here we explore the impact, of, i.e. damage caused by, temporarily varying plastic on predator-prey interactions. We quantify damage in terms of a cost function which measures both the amount of plastic and its impact. This then leads to a variety of optimisation problems which in turn furnish the “worst” i.e. most damaging temporal form of the plastic. Often we find that the most damaging plastic is ”on-off” - acting full-on at the worst time for the species interaction and switching off when the plastic-free interaction is bad for both species. Keywords: Plastic Pollution, Predator-Prey, Optimal Control.

ADAPTIVE CONTROL OF WAVE SPEED IN INTEGRAL PROJECTION MODELS OF INVASIVE PESTS

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Markus Mueller and Stuart Townley, Environment and Sustainability Institute, College of Engineering, Mathematics and Physical Sciences, University of Exeter, Penryn Campus, TR10 9FE.

Integral projection models (IPMs) can be used as models for spatio-temporal processes. Here we borrow ideas from Kot, Lewis, and van den Driessche, 1996, who used IPMs to model spatially distributed biological invasions. The speed of the biological invasion is a key property which may act as a proxy for the damage caused by the pest. The speed of invasion, or invasive wave speed, in the IPM depends on the form of the IPM kernel Gaussian and exponential distributions. These kernels depend on parameters which control the per-time-step spread of the pest. Parameters yielding narrower kernels lead to slower speed of spread. Now suppose we want to reduce the speed of spread (aka damage) to some below some pre-determined threshold. Assuming that increasing volume of pesticide narrows the kernel, we propose an adaptive algorithm which drives the speed to below the set threshold

using an estimate of current speed. We apply our results to the control of invasion speed in D.pseudoobscura.

Keywords: Integral projection models, adaptive control, spatially distribution, wave speed.

Velocity fields in a two-layer fluid with an interfacial solitary wave

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Loughborough University

Ricardo Barros and Karima Khusnutdinova, Loughborough University

We consider different model equations governing the evolution of internal gravity waves at the interface of two immiscible fluids between two rigid walls. Their solitary-wave solutions are examined and compared with those of the Miyata-Choi-Camassa (MCC) model, known to be in good agreement with the large amplitude wave profiles observed in laboratory experiments and numerical solutions for Euler equations. Knowing the velocity fields in the water column in the presence of such waves is useful for comparisons with experimental results obtained through particle imaging velocimetry (PIV), but also to determine the loads the waves can exert on structures. Keywords: Water waves, solitary waves, interfacial waves, asymptotic analysis, velocity fields, two-layer fluid

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Modelling the labour market: Can we predict occupation transitions?

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Understanding the impact of societal and economic change on the labour market is important for any cause, such as automation or the post-carbon transition. Occupational mobility plays a role in how these changes impact the labour market because of indirect effects, brought on by the different levels of direct impact felt by individual occupations. We present an agent-based model which uses a network representation of the labour market to understand these impacts. This network connects occupations that workers have transitioned between in the past, and captures the complex structure of relationships between occupations within the labour market. We develop these networks in both space and time using rich survey data to compare occupational mobility across the United States and through economic upturns and downturns to start understanding the factors that influence differences in occupational mobility. Finally we explore the potential for the model to predict occupational transitions. Keywords: Labour market; agent-based model; complexity economics; networks

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Spontaneous emergence of oscillatory behaviour in plastic dynamical systems

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"The complex and unique behaviours of the human brain present many challenges for scientists trying to recreate the dynamics of cognition in artificial systems: the brain simultaneously performs various cognitive processes such as pattern recognition, categorisation, memorisation, and forgetting, and develops in response to new environments. A novel class of dynamical system was introduced in [1] and further studied in [2,3] as a candidate model of an explainable intelligent system, inspired by the self-organised plasticity of the brain. To date, only the simplest gradient systems have been considered. Such systems are unable to reproduce qualitative phenomena observed in the biological brain, where neurons demonstrate oscillatory behaviour spontaneously. To overcome this, we propose a minimal model for the spontaneous emergence of oscillations in a controllable manner in dynamical systems with plastic and self-organising velocity vector fields.

[1] Janson, N.B., Marsden, C.J. Dynamical system with plastic self-organized velocity field as an alternative conceptual model of a cognitive system. Sci Rep **7**, 17007 (2017).

[2] Janson, N.B., Kloeden, P.E. Mathematical Consistency and Long-Term Behaviour of a Dynamical System with a Self-Organising Vector Field. J Dyn Diff Equat **34**, 63-78 (2020).

[3] Janson, N.B., Kloeden, P.E. Robustness of a dynamical systems model with a plastic self-organising vector field to noisy input signals. Eur. Phys. J. Plus **136**, 720 (2021).

Keywords: Non-autonomous dynamical systems, oscillations, bifurcations, self-organisation, stochastic processes

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Dynamics of swelling and shrinking thermo-responsive hydrogels

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Hydrogels are polymer networks that can absorb and retain large amounts of water, which can result in substantial swelling. Unlike most materials that expand upon heating, thermo-responsive hydrogels significantly reduce in volume in response to a temperature increase, as the polymer becomes more hydrophobic and expels water. Understanding the dynamic behaviour of such systems can be difficult because of the spatially- and temporally-varying properties of the gel, and the complex relationships between the elastic deformation of the polymer structure, the fluid dynamics within the pore spaces and chemical interaction between the polymer and fluid.

We investigate such a gel using a poro-elastic model, considering the dynamics of a homogeneous thermo-responsive spherical hydrogel after a sudden change in the temperature that should result in substantial swelling or shrinking. We typically find that swelling and shrinking have qualitatively different behaviour: swelling happens smoothly from the edge, whereas shrinking results in the formation of an inwards-travelling spherical front that separates a swollen core and shrunken shell. An approximate analytical form for the front dynamics is developed that well-approximates the numerical solutions. Keywords: Hydrogels, swelling, poro-elasticity

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Riemann problem for a dense soliton gas for the KdV equation: a numerical study

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We numerically realise the generalised Riemann problem for dense soliton gas of the Korteweg-de Vries (KdV) equation whereby soliton gas is prepared in different macroscopically homogeneous states on the left- and right-hand side of space. The emerging non-equilibrium dynamics are compared with the analytical predictions of the spectral kinetic theory of soliton gas. The numerical scheme is based on the construction of an appropriate exact N-soliton solution of the KdV equation with N large and random distribution of initial phases. Keywords: Korteweg-de Vries equation; soliton gas; Riemann problem

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Dynamics in a magnetic pendulum model: dipole-dipole interactions and chaos on a sphere

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In its most familiar incarnation, the magnetic pendulum comprises a magnetic bob that is free to swing in three-dimensional (3D) space. Below, a horizontal base-plane contains three similar magnets; each is arranged in the opposite-poles-attract configuration relative to the bob, and placed on the vertices of an equilateral triangle. Peitgen, Jürgens, and Saupe proposed in the early 1990s a phenomenological equation of motion for a magnetic pendulum with two degrees of freedom [Chaos and Fractals: New Frontiers in Science, Springer, 1992]. Their approach was to adopt a plan view of the pendulum, using Cartesian coordinates and a 2D damped simple harmonic oscillator (SHO) to represent a projection of the bob's position as it darts erratically to-and-fro above the base-plane magnets. Linear damping was accommodated by including a drag force proportional to negative velocity. Moreover, the magnetic interactions were assumed to originate from point sources which led naturally to an inverse-square force law. This toy model is appealing in its simplicity, though analysis by Motter et al. [Phys. Rev. Lett., vol. 111(19), art. no. 194101 (2013)] uncovered surprisingly rich behaviours. However, the damped-SHO paradigm and its ad hoc inverse-square rule mimicking magnetism does not provide an entirely satisfactory picture of the real system. Here, a more physical model is proposed for the magnetic pendulum. At the outset, the problem is formulated by deploying Lagrangian dynamics. The bob, in reality, moves through space along the surface of a sphere whose centre coincides with the suspension point and whose constant radius provides a holonomic constraint. Hence, the natural coordinates to use turn out to be the azimuthal and polar angles. The restoring force of gravity is straightforward to include, and linear damping is introduced through a velocity-dependent potential. Crucially, magnetic dipole-dipole interactions, which have an intrinsic directional character replace the assumption of inverse-square attraction. In these ways, the classic model changes non-trivially from the damped SHO-type to the damped spherical pendulum-type. This presentation will look at the derivation and scaling of the governing equations, which are somewhat complicated in structure and computationally expensive to solve. There appear several additional quantities that must be specified in order to fully characterize the pendulum, increasing dramatically the size of the parameter space. The phenomenon of sensitive dependence on initial conditions will be demonstrated. Preliminary computations of the basins of attraction will also be shown, providing some qualitative evidence of fractality in the structure of their boundaries. Keywords: Chaos, fractals, magnetism, nonlinear dynamics.

Minimum information variability via model predictive control

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When studying complex systems, using mathematical descriptions via time-varying probability density functions (PDFs) has become a practical approach that permits us to consider different control engineering problems. For instance, the regulation (set to a fixed value) or tracking (follow a path) of the PDF's time evolution, now viable for applications such as colloidal systems thanks to optical tweezers. The proposed poster illustrates a solution based on Model Predictive Control (MPC) and Information Geometry. Specifically, it discusses an online optimisation method to minimise the information length's metric of the system's probability distribution through time. Additionally, it analyses the effects on the system's entropy production and entropy rate under the closed-loop method. The algorithm is tested numerically in the Ornstein-Uhlenbeck process to demonstrate its feasibility. Keywords: Stochastic thermodynamics; control systems; Fokker Planck equation; Model Predictive Control

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Estimating critical power in cycling from routinely collected training data

Jonah Drake

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The critical-power model is widely used by cyclists to assess and track their fitness. Unfortunately, the current approach for learning its parameters requires a so-called "critical-power test" which strenuous on the rider and thus only carried out infrequently. We present a method for learning the model parameters from data that cyclists already routinely collect during training rides. Keywords: critical power; parameter estimation; cycling.

Optimisation of an elastic filament for propulsion in viscous fluid

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Eric Lauga (Department of Applied Mathematics and Theoretical Physics, University of Cambridge)

The oscillations of an elastic slender filament are used as a mode of swimming by many eukaryotic cells, thus inspiring the design of various artificial micro-swimmers. The time-varying shape of this elastic filament is what determines it propulsion efficiency in a viscous fluid, and that shape depends critically on the spatial distribution of the bending rigidity (BR) along the filament. In this work, we optimise theoretically the spatial distribution of BR to maximise the propulsive force of the filament. We consider a slender elastic filament that oscillates in a viscous fluid at small amplitude. The governing equations for the evolution of the shape of the filament in time are derived using the balance of viscous and elastic forces; for small amplitude oscillations this is the classical linear elasto-hydrodynamic equation. The BR, which governs the magnitude of the elastic force, is assumed to be an arbitrary function of space. We formulate an optimization problem that maximises the propulsive force with respect to the BR function. The functional derivative of the propulsive force with respect to BR is obtained using an adjoint problem and we solve the functional optimisation problem numerically via a steepest descent algorithm in functional space. We consider two sets of additional constraints: (i) a bounded BR function or (ii) a fixed volume of the filament. In the case of bounded BR, we find that the optimal shape obtained from our simulations is a step function, which takes the value of the upper bound near the base of the filament and the value of the lower one at its distal end. The propulsion is therefore maximised if the base of the filament is very stiff while the distal end is soft, with a propulsive force that increases up to four times when compared to the case of a spatially homogeneous BR. Our results suggest the choice of material and/or shape of the filament that propels most efficiently in viscous fluids and may help the design of future artificial swimmers.

Keywords: low Reynolds number swimming, linear elasto-hydrodynamics, functional optimisation

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Asymptotic model for rolling

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99% of steel, and 2/3 of aluminium, are rolled into sheets as the first step of being used in manufacturing. Given the high capital cost of a modern production mill (on the order of USD 100 million), any small improvement to the current forming process is worth considering. There is currently interest within manufacturing in real-time online control of metal forming, and an identified need for sufficiently-accurate quick-to-compute models. Here, we focus on the evolution of texture and anisotropy during strip metal rolling. We describe a recent asymptotic mathematical model for rolling based on a rigid perfectly-plastic material model, and propose some extensions to include a more sophisticated material model, including strain hardening and the development of anisotropy.

Keywords: Rolling-Asymptotic analysis-Texture- Anisotropy

Exploring Artificial Neural Networks as Dynamical Systems

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The results in this presentation illustrate some of the early phases of exploration into the field of artificial neural networks from the viewpoint of dynamical systems. In particular, this research was conducted by utilising some of the common analytical and numerical techniques used in the study of ordinary differential equations and dynamical systems such as phase-plane analysis, Velocity Vector fields and Bifurcation theory. The neural networks in this presentation range from simple 2 & 3 neuron models to 81 neuron models in a single layer network. The simplicity of the 2&3 neuron models allows us to more easily visualise aspects of our system such as the 2/3 dimensional state space of neuronal activities, however, a caveat to this is that this small number of neurons does appear to limit the capabilities of the neural network itself and hinder its ability to learn and perform pattern recognition. On the contrary, an 81-dimensional network can seemingly perform simple pattern recognition given sufficient time to learn but unfortunately due to its nature, visualising the 81-dimensional state space, basins of attraction and Locations of attractors themselves is much more challenging. So far the best approach has been to observe projections of these 81-dimensional spaces onto the plane, or in some case, 3 dimensions or to take 2&3 dimensional hyper surfaces within our space. The aim of this work has been to establish whether viewing these neural networks from a dynamical systems perspective may provide us with a clearer picture on the process of learning, the stability of these systems in relation to undergoing bifurcations and the tendency for errors to occur in pattern recognition post-learning.

Keywords: Dynamical systems; Artificial Intelligence

The combinatorial structure of determinantal systems for Groebner basis computation: Critical values and beyond

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Alin Bostan, Jérémy Berthomieu, Huu Phuoc Le, Mohab Safey El Din

Determinantal ideals generated by the minors of polynomial matrices arise in a wide variety of domains including cryptography, polynomial optimisation and effective algebraic geometry. A case of particular importance is when the determinantal ideal is generated by maximal minors as such ideals model encode many problems. By the Jacobian criterion, the set of critical values of a polynomial restricted to a smooth algebraic set can be represented in this way. Hence, we aim to understand how the determinantal structure affects computations. Computing Gr"obner bases is a classical and efficient method for solving polynomial systems. A popular method in practice is to first compute a Gr"obner basis with respect to a term order favourable for computation, such as a degree reverse lexicographic ordering. Then, one can apply a change-of-ordering algorithm to find a Gr"obner basis of the same ideal but with respect to the desired term order. For example, a lexicographic ordering which, under some genericity conditions, gives a triangular representation of the set of solutions, an analogue of Gaussian elimination in our non-linear framework. When the solution set is finite, a fast algorithm for this change-of-ordering step is Sparse-FGLM by Faugère and Mou. The complexity of this algorithm is $O(mD^2)$, where D is the number of solutions and m is the number of dense columns of a certain sparse, structured $D \times D$ matrix. Under Moreno-Socías' conjecture, the number m was analysed by Faugére and Mou in the case of generic ideals. By assuming variants of Fr"oberg's conjecture, we continue this line by finding asymptotic estimates for m in the case of determinantal systems deriving from maximal minors and in particular those encoding critical values. This is accomplished by relating m to the coefficients of the Hilbert series of these systems. Moreover, we prove an upper bound on the complexity of the change-of-ordering step for general determinantal systems. When the matrix in question is symmetric, the Hilbert series of the resulting determinantal system is known for certain sizes of minors. In these cases, we give finer complexity estimates than what was known from general bounds. Experimental results are given to support our asymptotic bounds and the conjectures upon which our results rely. Joint work with Alin Bostan, Jérémy Berthomieu, Huu Phuoc Le and Mohab Safey El Din.

Keywords: Groebner bases, critical values, determinantal systems, FGLM, combinatorial commutative algebra, applied algebraic geometry

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A stochastic model of the L-H transition in fusion plasma

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The Low-to-High confinement (L-H) transition is an extremely important phenomenon in magnetic confinement fusion (MCF) research. It involves a sudden improvement in the confinement conditions of a fusion device when an input power threshold is reached. The work here presents a stochastic prey-predator model of the L-H transition. The model involves the interplay of turbulence, zonal flow shear, mean flow shear and the (ion) pressure gradient. The (transformed) turbulence and zonal flow shear are treated as stochastic variables and a corresponding Fokker-Planck equation for the time-dependent probability density function (PDF) is solved numerically. As well as studying the time evolution of the PDF, information length and entropy diagnostics are employed to study the changes to the system and the environment. Hysteresis associated with the L-H transition and its backward, H-L transition is studied by using three input power functions, which are symmetric around a time t_*. The results highlight the importance of non-Gaussian PDFs and time-varying fluctuations in the transitions.

Keywords: L-H transition, stochastic, Fokker-Planck, information length, non-Gaussian PDF, hysteresis

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Magnetic helicity and field linkage in spherical dynamos

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Magnetic helicity is a measurement of field line entanglement weighted by magnetic flux. On the Sun and other stars, magnetic helicity density at the stellar surface is used as a proxy for the internal behaviour of the dynamo driving the global magnetic field. In this note, we study the behaviour of the global relative magnetic helicity in spherical dynamos. We also investigate a related quantity, the global linkage, which is a renormalized form of relative magnetic helicity that removes the field strength weighting and provides a direct measure of field linkage. The behaviour of these topological quantities is described for different types of the dynamo. The results shed light on how magnetic helicity observations can be used to interpret global dynamo behaviour.

Keywords: magnetohydrodynamics, magnetic helicity, dynamo

Dynamical minimum action paths and non-equilibrium transitions

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The time evolution of many physical, chemical, and biological systems can be modelled by stochastic transitions between the minima of the potential energy surface describing the system of interest. Various techniques to compute the minimum energy (and hence most probable) path between two minima exist, including the string method (SM [1]) and the geometric minimum action method (gMAM [2]). Such paths are everywhere parallel to the potential gradient, and correspond to the infinite-time transition. In this work, we extend the approach to finite-time transitions, and use a modified gMAM method to compute finite-time, out-of-equilibrium paths. These are no longer parallel to the potential gradient, and correspond to the most probable path conditioned on a finite duration. We explain how these paths are connected to the full transient dynamics of the system, as described by the time-dependent Fokker-Planck equation.

[1] W E W Ren and E Vanden-Eijnden, J. Chem. Phys. 126 (2007): 164103
[2] E Vanden-Eijnden and M Heymann, J. Chem. Phys. 128.6 (2008): 061103
(Leines and Rogal, Phys. Rev. E 93, 022307 (2016))

Keywords: Non-equilibrium dynamics; path integrals; stochastic processes

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Continuum scale modelling of blood flow in sickle cell disease

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Particle suspensions in confined geometries exhibit rich dynamics, including flowing, jamming, and clogging. Such effects can be an important determinant of function in blood flow affected by malaria or sickle cell disease. The aim of this work is to shed light on the macroscopic dynamics of particle suspensions in the context of these diseases. To this end, we develop continuum mathematical models of particle suspensions that account for spatio-temporally varying material properties. The results will improve our understanding of how particle-scale physical processes in non-Newtonian fluids can be captured using mathematical models at the continuum scale. Keywords: Sickle cell disease, Non newtonian fluid, continuum scale modelling, Herschel-Bulkley model, Particle suspensions

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A higher order virtual element method for the Cahn-Hilliard equation

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In this work we discuss nonconforming virtual element methods (VEMs) for fourth-order problems. The construction of even a lowest order C^1 conforming space is not straightforward within the standard finite element setting and higher order nonconforming spaces suitable for fourth-order problems are also not readily available. At present, the available VEM literature on fourth-order problems only includes defining projection operators based on the underlying variational problem. This approach involves constructing only one projection which depends on the local contribution to the bilinear form. Instead, we follow the approach of defining a hierarchy of projection operators for the necessary derivatives with the starting point being a constraint least squares problem. By defining the projection operators in this way we show that we can directly apply our method to nonlinear fourth-order problems. This approach can also be easily included into existing software frameworks. This poster discusses the application of our generalised method to the Cahn-Hilliard equation. As a consequence of our approach, we do not require any special treatment of the nonlinearity. Our method is shown to converge with optimal order also in the higher order setting. The theoretical convergence result is verified numerically with standard benchmark tests from the literature.

Keywords: Numerical analysis, numerical methods for PDEs, polygonal methods, virtual element method, Cahn-Hilliard equation, nonlinear fourth-order problems

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First passage time densities from stochastic path integrals

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Dr Steve Fitzgerald, University of Leeds

Many fluctuation-driven systems have important events that occur when a stochastic process encounters a boundary for the first time, e.g. barrier-crossing in chemical kinetics, integrate-and-fire models for neurons, or the triggering of certain options in finance. [1] The Fokker-Planck equation can in principle be used to find the first passage time densities for these occurrences. However, this can only be done numerically except for the simplest systems, and quickly becomes computationally intractable as the number of dimensions increases. In this work, we investigate how path integrals [2] can be used to find an approximate analytical form for the first passage time density for diffusion in a nonzero potential. We derive this form for a sloped potential in one dimension with both absorbing and reflecting boundary conditions, and discuss generalisations to higher dimensions and more complex potentials.

[1] S. Redner. A Guide to First-Passage Processes. A Guide to First-passage Processes. Cambridge University Press, 2001. isbn: 9780521652483.

[2] H.S. Wio. Path Integrals For Stochastic Processes: An Introduction. World Scientific Publishing Company, 2013. isbn: 9789814449052.

Keywords: First passage problems, Path Integrals

Nonlinear acoustics in a general 3D duct

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University of Warwick

Ed Brambley, University of Warwick

The aim of this project is to reproduce and build upon the work of McTavish, J. P. (2019) in modelling nonlinear sound propagation in 3D waveguides, with an application to the harmonic series of brass instruments. Time-harmonic perturbations about a state of rest are considered up to second order (weak nonlinearity). The governing equations for weakly nonlinear sound are then projected onto a basis of straight, cylindrical duct modes before the consideration of the duct outlet physics. Eventually the impedance along the duct is calculated for various geometries and endpoint conditions; this can be informative as to the harmonic series of a brass instrument, for example. Keywords: Acoustics

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Are there purely topological explanations of the number of equilibria of pendulum systems?

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University of Canterbury, New Zealand

Phillip Wilson, Douglas Campbell and Clemency Montelle

Distinctively topological explanations (DPE) of physical systems bypass their complex dynamics and explain certain physical features of these systems that remain invariant (as a topological constraint on the system) despite a considerable change in their dynamics. Lange (2016) provides one such explanation of a constraint on the minimum number of equilibria of double pendulums. He shows that one can map the potential energy (P.E.) function of the double pendulum onto its configuration space, a torus, and reason about the number of critical points of this mapping (a distorted torus) to get a global constraint on the minimum number of its equilibria. This is because such mappings are generally homoeomorphic and obey the Morse inequalities. This talk refutes both Lange's claim itself and a strengthened and extended version of the claim, involving Betti numbers of the distorted configuration space (an n-torus), that would pertain to any n-tuple pendulum system showing there are no topological constraints on the number of equilibrium positions of any n-tuple pendulums. The talk shows how such explanations fail generally for non-Morse P.E. functions when perturbations are introduced in the length of the pendulum rod in such a way that: (a) one or more critical points of the P.E.

function become degenerate (or badly degenerate), which makes it difficult (and in some cases impossible) to ascertain the index of these degenerate critical points, and/or (b) the P.E. function may no longer be mappable to a smooth or compact manifold, and thus Morse inequalities fail to be applicable. The talk then briefly considers workarounds or extensions of Morse theory (Bartsch et al. 2008; Bismut 1986; Popescu 2004; Witten 1982), including the notable Catastrophe theory (Castrigiano & Hayes 2019), that deal with a general theoretical framework to handle degenerate points, but shows them to be inadequate to handle the objections raised above. The arguments in the paper generalise for any dynamical system with a purported DPE analogous to the one proposed by Lange.

References: Bartsch, T., Szulkin, A., M., W. (2008). Morse theory and nonlinear differential equations. D. Krupka & D. Saunders (Eds.), Handbook of global analysis (pp. 41-73). Amsterdam: Elsevier. https://doi.org/10.1016 B978-044452833-9.50003-6 Bismut, J. (1986). The witten complex and the degenerate morse inequalities. Journal of Differential Geometry, 23(3), 207-240. 10.4310/jdg/1214440113 Castrigiano, D., & Hayes, S. (2019). Catastrophe theory. CRC Press: Taylor & Francis Group. 10.1201/9780429501807 Popescu, I. (2004). Morse inequalities, a probabilistic approach (Unpublished doctoral dissertation). MIT.

Keywords: Oscillating systems; Applied Topology; Perturbation analysis

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Ice particle skimming in the aircraft icing context

Ellen M Jolley
UCL
Frank T Smith

As an air vehicle flies through cloud at temperatures below freezing, it encounters ice particles and supercooled droplets which result in the accretion of ice onto the vehicle surfaces and hence the deformation of its aerodynamic shape. This can, in worst cases, cause series accidents (Gent, 2001). The study of the dynamics of such particles is thus essential to developing effective icing protection systems. The problem is complex because of (among other things) the wide range of sizes and shapes of possible particles. In the work presented here, we focus on tackling the situation where there is a thin layer of water on the aircraft surface (as can happen in icing scenarios) and the particles are similarly thin such as to be able to interact with the water layer. The result is a wide range of possible motions of the particle, including both sink cases (the particle enters the water and becomes submerged) and skim cases (where the particle is launched back off the surface of the water following contact). The latter case has analogy with traditional stone skimming/skipping games found around the world. The technique which has allowed us to make significant headway with this problem has been to study surface fluid layers of arbitrary density (hence including fluids with density similar to that of the air), which however can then be used to study the water case by taking the layer fluid density to be approximately one thousand times that of the air. As well as aiding progress with the water case, this model has the significant benefit of being more general and thus applicable to a wider range of scenarios. Under suitable assumptions (including that the body and the layer are thin, that the Reynolds and Froude numbers are large, and that the body is much denser than the air) the model allows the shape of the layer interface and pressure profile beneath the body to be calculated for a given body position. This in turn allows the forces on the body to be calculated and hence for the motion of the particle to be computed in full, revealing the aforementioned sink and skim behaviours. For cases where the body is heavier than both the air and the liquid layer (and hence affected by gravity), the repeated skims familiar to many through childhood games are found.

Keywords: fluid-particle interaction; multiphase flow; asymptotic analysis; nonlinear dynamics; aerodynamics

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Crime and neighbourhoods, or how the community's actions affect crime rates

Laura Jones
University of Surrey

What if residents of a neighbourhood could influence crime rates by their behaviour? This is what postulates the theory of collective efficacy. Collective efficacy is the conviction shared by a group of people that they can work together to successfully complete a specific task. The idea is that the difference in neighbourhoods iinner structure leads to spatial variation in crime rates. Many models exist that show the negative link between collective efficacy and crime but the literature in studying the formation of patterns is still limited. We present a novel convolution model of collective efficacy that allows for a mathematical investigation of neighbourhood and resource effects on the formation of collective efficacy and transitions between different regions of collective efficacy.

Keywords: criminology; hotspots formation; convolution product; Fourier transform

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Optimising antibiotic release from medical implants to counteract biofilm formation

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Nigel J. Mottram, School of Mathematics and Statistics, University of Glasgow; Sean McGinty, James Watt School of Engineering, University of Glasgow.

Biofilms are aggregations of microorganisms that attach to surface and which can be associated with a variety of persistent and device-centered infections. Implant infection can lead to chronic pain which , when severe may lead to amputation to protect against life-threatening sepsis. One possible solution would be the administration of antibiotics, preferably targeted to a specific location. We have formulated a model in which we introduce controlled antibiotic release directly from the implant

in order to consider delivery strategies. If the release is inadequate to prevent bacterial growth then infection can take hold, however if drug release is excessive then this may impair the recovery of healthy tissue around the implant. The approach of modelling biofilm growth while optimising antibiotic dose and release rate simultaneously may result in a more efficient biofilm eradication strategy. In stage-I of this investigation, a mathematical model concerning only the growth of a matured biofilm on an implant is considered. In stage II, we introduce a mathematical model which also includes eradication of infection by releasing antibiotics from an implant. The stage-I model consists of active bacteria, self-produced extra cellular polymeric substance (EPS), nutrient, water volume fraction and movement of the biofilm [1]. Here, the metabolic rate of bacteria follows Monod kinetics together with a natural death rate. No-flux conditions for bacteria, nutrient and EPS are applied at the implant surface and a Dirichlet condition is applied at the moving boundary to capture a constant influx from a external bacteria-laden environment. The model in stage-II is an extension of the Stage-I model with the additional consideration of persister bacteria, dead bacteria and the release of antibiotic from the implant [2]. In this model, antibiotic-induced death of active bacteria along with natural death and the conversion from active bacteria to persister bacteria and vice-versa are considered. The governing partial differential equations are then solved using Matlab. One intriguing observation is that the diffusivity of the nutrient and the nutrient consumption rate both affect the advection velocity, and control the growth and maturation of the biofilm. Simulations also predict that the local release of antibiotic dose counteract the growth of biofilm by reducing the growth of active bacteria, and an appropriate therapeutic dose will help in eradicating it.

[1] F. Abbas, R. Sudarsan, and H.J. Eberl. Mathematical Biosciences and Engineering, 9(2):215, 2012.

[2] J.K. Miller, J.S. Brantner, C. Clemons, et al. Mathematical Medicine and Biology: a Journal of the IMA, 31(2):179-204, 2014.

Keywords: biofilm formation; medical implants; antibiotic release.

Stability, Collapse and Hyper-chaos in a Tri-Trophic Predator Prey model with Mutation and Predation

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We present a set of four three dimensional models (basal food source - prey - predator) all with variations in the predator's behaviour. The main focus is the effect of the basal food source consumption on the stability of the ecosystem with the presence of mutation and predation. Various behaviours are presented including chaotic and hyper-chaotic behaviour which are calculated using the Lyapunov exponents. We find that increased consumption is beneficial for some of our models whilst being detrimental to others. In all of the models, increased consumption reduces the extent to which over-predation leads to extinction of the prey. Mutation was found to have a larger impact in stability if the mutant is an omnivore, with no chaotic behaviour occurring in certain regions of parameter space.

Keywords: Chaotic Dynamics; Lyapunov Exponents; Three-dimensional models

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Non-spherical form factors in Crystallography

Laura Midgley

Durham University

L. J. Bourhis, O. V. Dolomanov, S. Grabowsky, F. Kleemiss, H. Puschmann and N. Peyerimhoff

Early crystallographers needed to simplify the theory behind crystallography for ease of calculation, and did so by pre-calculating tables of scattering power ('form factors') for atom types based on individual atoms without bonds or interaction - the 'independent atom model', or IAM. With the growth of modern computing and quantum-mechanical modelling software, we are now able to directly calculate electron densities and scattering patterns of specific molecular arrangements, and thus have more accurate form factors for atoms within molecules. Much crystallographic theory holds up well when we move from the pre-tabulated constant form factors to the changeable molecule-dependant form factors. However, during structure refinement utilising least-squares refinement we rely on derivatives - including the partial derivatives of these form factors. In the independent atom model, the form factors themselves did not change with molecular changes, and so this derivative was 0. However, with the new method, these form factors will change as the molecule does. The complexity of quantum mechanical calculations means that this derivative is very difficult, if not impossible, to calculate exactly. I tested the impact of instead allowing this derivative to remain estimated at zero within the least-squares process, using numerical differentiation to determine the actual derivative and refine correctly with that. I found that the resulting structures when correctly refined were within the current measurement uncertainty for crystallography, and thus there is currently no issue with crystallographic software discarding these form factor derivatives, which is very costly to determine.

Keywords: Crystallography, X-ray diffraction, nonspherical form factors, least squares minimisation

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The implementation of resolved interfaces in a bubble-scale model for gas diffusion in wet foams

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Foams, which comprise packings of gas bubbles separated by a liquid phase, are not stable. Pressure differences between the bubbles drive gas diffusion through the liquid, causing large bubbles to grow while small ones disappear, even in the absence of merging events due to the bursting of liquid films. This process is termed coarsening, and questions remain regarding its consequences when the foam's liquid fraction (the volume of liquid per unit volume of the foam) lies between the limiting cases of zero (corresponding to dry foams with bubbles separated by infinitesimal films) and one (the wet limit, comprising isolated bubbles, infinitely far apart). How does the mean bubble radius vary with time, and, relatedly, how can gas diffusion rates be predicted when films coexist with thicker collections of liquid (Plateau borders)? Due to the structural complexity of foams, an important mode of theoretical investigation on the bubble scale is through numerical models. However, realistic finite-element simulations of coarsening wet foams have been difficult, particularly in three dimensions, due to the need to adjust the discretisation during the foam's structural transitions - a consequence of treating the liquid films as having zero thickness. Systematic studies in this regime have therefore used idealised models, and have not yet quantitatively reproduced existing experimental results concerning the above questions. However, a different approach, thus far applied to foam rheology in two dimensions, may bring improved simulations of this process. This allows structural transitions to occur naturally by modelling arbitrarily-shaped bubbles which interact through disjoining pressure [Kähärä et al (2014). Phys Rev E. 90: 032307], the mainly repulsive interaction between opposing liquid-gas interfaces that stabilises the liquid films. Hence, every liquid-gas interface is resolved. We present a new model of this type, intended for simulations of coarsening wet foams, which makes use of the Surface Evolver [Brakke (1992). Exp Math. 1: 141]. A focus on quasi-static dynamics allows the application of its efficient algorithms for energy minimisation. We also implement a realistic form for the disjoining pressure, allowing its attractive component to be varied, together with a bespoke nearest-neighbour algorithm to determine the film thicknesses. In order to test this model, we compare its predictions of the static shear modulus for various ordered foams with existing theoretical results.

Keywords: foams, complex fluids, diffusion, thin films, numerical modelling

Newtonian and non-Newtonian Slippery Liquid Infused Porous Surfaces using the lattice-Boltzmann algorithm

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Dr Ciro Semprebon, Northumbria University

Slippery Liquid-Infused Porous Surfaces (SLIPS) coating consist of a nano/micro-structured porous material infused with a lubricant fluid. When a droplet is deposited on a SLIPS, the lubricant prevents most of the contact of liquids with the underlying solid, thus virtually suppressing the friction forces arising from contact line pinning [1]. Consequently, by hindering the material defects and imperfections, SLIPS provide a unique approach to coating surfaces for more precise tuning of the fluid properties, with the advantage of reducing the solid contamination by repelling almost any fouling challenge a surface may face, for example from bacteria. We investigate the interplay of the lubricant (Newtonian/non-Newtonian) on the droplet behaviour. We use a lattice Boltzmann algorithm based on a ternary model on SLIPS for the lubricant and the droplet recently developed within our group [3], implementing a strain-rate dependent viscosity and investigating the motion of non-Newtonian liquids on both simple and complex lubricants. Our goal is to gain insight into this system at a fundamental level, to inform the design of experiments. We study the SLIP behaviour under actuation by external forces by quantifying the dissipative forces and by measuring the response of the apparent contact angle of a droplet when actuated by a body force.

[1] F Schellenberger, et al., Soft Matter, 2015,11, 7617-7626.

[2] M S Sadullah et al., Langmuir 2018, 34, 8112-8119.

[3] J Boyd et al., Phys. Fluids 19, 093103 (2007).

Keywords: wetting, capillarity, fluid-dynamics

GParareal: A time-parallel ODE solver using Gaussian process emulation

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Sequential numerical methods for integrating initial value problems (IVPs) can be prohibitively expensive when high numerical accuracy is required over the entire interval of integration. One remedy is to integrate in a parallel fashion, “predicting” the solution serially using a cheap (coarse) solver and “correcting” these values using an expensive (fine) solver that runs in parallel on a number of temporal subintervals. In this work, we propose a time-parallel algorithm (GParareal) that solves IVPs by modelling the correction term, i.e. the difference between fine and coarse solutions, using a Gaussian process emulator. This approach compares favourably with the classic *parareal* algorithm and we demonstrate, on a number of IVPs, that

GParareal can converge in fewer iterations than parareal, leading to an increase in parallel speed-up. GParareal also manages to locate solutions to certain IVPs where parareal fails and has the additional advantage of being able to use archives of legacy solutions, e.g. solutions from prior runs of the IVP for different initial conditions, to further accelerate convergence of the method - something that existing time-parallel methods cannot do.

Keywords: Parallel-in-time, Gaussian process emulation, parareal, initial value problems

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Mathematical modelling of protein aggregation in sickle cell disease

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Dr Philip Pearce (UCL), and Dr Thomas Michaels (UCL)

Sickle cell disease is a genetic blood disorder induced by the polymerization of sickle haemoglobin (HbS) inside red blood cells (RBCs) in reduced oxygen tension. Polymerization causes RBCs to become stiffer, increasing effective blood viscosity and contributing to occlusion of blood vessels. As a first step to develop a multiscale model of HbS polymerisation, we present here various mathematical frameworks for the length distribution of biopolymers.

Keywords: kinetic theory, sickle cell disease, biomathematical modelling

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Numerical spectral synthesis of soliton and breather gas

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P. Suret and S. Randoux, Université de Lille; G. El and T. Congy, Northumbria University

Soliton gas was introduced by Zakharov [Sov. Phys. JETP **33**, 538 (1971)] as an infinite ensemble of interacting KdV solitons randomly distributed in velocity and positions. This concept has been extended by El and Tovbis [PRE, **101**, 052207 (2020)], in their development of the spectral theory of soliton and breather gases, in the framework of the focusing Nonlinear Schrodinger (fNLS) equation. Moreover, it has been shown in a recent work by Gelash et al. [PRL, **123**, 234102 (2019)] how the spectral soliton gas formalism could lead to a new understanding of the evolution of random processes in integrable systems, the so-called integrable turbulence. In this context, the ability to numerically build the soliton and breather gas solutions from the nonlinear spectral plane is a key element for testing the mathematical model and investigating its physical applications. In this work, we present the algorithms for the synthesis of soliton and breather gases in the KdV and fNLS framework and we discuss the theoretical and numerical challenges that arise in the implementation. This is joint work with P. Suret, S. Randoux, G. El and T. Congy.

Keywords: Soliton Gas, Breather Gas, Spectral Theory, Spectral Engineering, Nonlinear Spectral Synthesis, IST, KdV, NLS

Rare events in turbulent fluid flows

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Tobias Grafke

Fluid in its turbulent state is one of the most complex interacting systems in physics, with an incredibly large number of strongly and nonlinearly interacting degrees of freedom. This becomes different when scale separation introduces coherent, long-lived structures into the fluid flow, which induces order and stability. We look at turbulent atmospheres of Jovian planets whose flows lead to coherent large-scale jets that persist for long times. These jets may be steady or transition between several meta-stable jet configurations which are driven by turbulent fluctuations. This work considers the stochastically forced barotropic two-dimensional quasigeostrophic equations in the β-plane, a classical two-dimensional model for the Jovian atmosphere. Direct numerical simulation of the quasi-linear approximation of this system is presented with verification of large time-scale separation between the slow zonal evolution and fast vorticity fluctuations. We exploit the time-scale separation property between these structures in the flow and apply the classical tool of stochastic averaging to obtain a closed limiting equation for the zonal evolution while averaging out the non-zonal fluctuations in the turbulent inertial regime $\nu \ll \alpha \ll 1$. The much simpler deterministic system allows us to analyse these meta-stable states, their basins of attraction, separating hypersurfaces, transition states and most likely transition trajectories from the perspective of bifurcation theory and large deviation theory. This is all carried out to answer the main question of under what conditions, and from what mechanisms, as well as with what probability can the system transition? i.e. how likely is it that Jupiter loses one of its jets?

Keywords: Geostrophic turbulence, Non-equilibrium steady states, Atmosphere dynamics, Limit theorems, Rare events

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The Role of the Double-Layer Potential in Regularised Stokeslet Models of Self-Propulsion

David Smith
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Meurig T. Gallagher, Rudi Schuech, Thomas D. Montenegro-Johnson

The method of regularised stokeslets is widely used to model microscale biological propulsion. The method is usually implemented with only the single-layer potential, the double-layer potential being neglected, despite this formulation often not being justified a priori due to nonrigid surface deformation. We describe a meshless approach enabling the inclusion of the double layer which is applied to several Stokes flow problems in which neglect of the double layer is not strictly valid: the drag on a spherical droplet with partial-slip boundary condition, swimming velocity and rate of working of a force-free spherical squirmer, and trajectory, swimmer-generated flow and rate of working of undulatory swimmers of varying slenderness. The resistance

problem is solved accurately with modest discretisation on a notebook computer with the inclusion of the double layer ranging from no-slip to free-slip limits; the neglect of the double-layer potential results in up to 24% error, confirming the importance of the double layer in applications such as nanofluidics, in which partial slip may occur. The squirming swimmer problem is also solved for both velocity and rate of working to within a small percent error when the double-layer potential is included, but the error in the rate of working is above 250% when the double layer is neglected. The undulating swimmer problem by contrast produces a very similar value of the velocity and rate of working for both slender and nonslender swimmers, whether or not the double layer is included, which may be due to the deformations locally rigid body nature, providing empirical evidence that its neglect may be reasonable in many problems of interest. The inclusion of the double layer enables us to confirm robustly that slenderness provides major advantages in efficient motility despite minimal qualitative changes to the flow field and force distribution.

Keywords: biological fluid mechanics, self-propulsion, computational methods, Stokes flow

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Fourier extensions for solving BVPs in one and two dimensions

Ghadeer Surrati

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Fourier series play an important role when we approximate analytic and periodic functions. For these functions, the Fourier series converges exponentially fast. In the case of non-periodic functions, this changes due to the Gibbs phenomenon. The Fourier extension technique can overcome the Gibbs phenomenon and lead to effective methods with spectral convergence in practice. In this technique, the non-periodic function defined on $[1, 1]$ is extended to a periodic function on $[T, T]$ with $T > 1$. Thus a periodic function defined on the larger interval is approximated by its Fourier series. Fourier extension can be used to solve BVPs with non-periodic BCs on any interval in 1D or an arbitrary domain in 2D. Keywords: Numerical methods - Fourier extension - non-periodic BVPs - Spectral methods.

Information Geometry from Stochastic Simulations

Abhiram Anand Thiruthummal
Coventry University

Stochastic Differential Equations (SDEs) are used to model a wide range of phenomena like cancer growth, chemical interactions, and stock prices. Although mean values and variance are often calculated and used to gain a key insight into these phenomena, they are not appropriate in describing large fluctuations where a significant deviation from mean values occurs. Furthermore, stationary probability distributions miss crucial information about the dynamics. One method of calculating the time evolution of probability distribution is to numerically solve the Fokker-Planck (partial differential) equation, which is computationally expensive and requires careful choice of boundary conditions. In this talk, we present an alternate Monte Carlo method to compute the probability distribution and associated statistics with the help of GPU-based large-scale parallel simulations. In particular, using Monte Carlo simulations, we investigate the time-evolution of nonlinear stochastic systems and elucidate its information geometry, which is the application of differential geometry to probability and statistics. Specifically, we calculate the information length [1] (path-dependent information geometry), which quantifies the information changes the system undergoes in time. New numerical algorithms are developed to accurately measure the information length from simulations. As a specific example, we present the information geometry of the attractor structure of different nonlinear dynamical systems.

[1] Kim, Eun-jin. "Information Geometry, Fluctuations, Non-Equilibrium Thermodynamics, and Geodesics in Complex Systems." Entropy 23.11 (2021): 1393.

Keywords: information geometry, simulation, monte carlo, stochastic differential equation, non-linear dynamics, GPU computing

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A Lagrangian perspective on integrability

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Most nonlinear differential equations produce dynamics that are hard to understand and impossible to solve explicitly. An exception are integrable systems, which are tamed by some underlying structure. Often, this structure consists of a number of symmetries. Each symmetry, in it infinitesimal form, defines a differential equation. These can be taken together with the original equation to form a system of differential equations. Hence we can argue that an equation is integrable if it is part of a sufficiently large family of compatible equations. Traditionally, the notion of "compatible" is made precise using Hamiltonian mechanics. This poster presents a lesser-known Lagrangian perspective on integrability. We characterise integrability using a variational principle, which can be applied far beyond the scope of mechanics, for example to integrable PDEs and discrete-time systems.

Keywords: Integrable systems, mathematical physics

Solute exchange in the umbilical cord

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The umbilical cord plays a critical role in delivering nutrients and oxygen from the placenta to the fetus through the umbilical vein while the two umbilical arteries carry deoxygenated blood with waste products back to the placenta. Solute exchange in the placenta has been studied widely, however the exchange within the cord tissue has not been investigated. The complex coiled structure of the umbilical cord could strengthen coupling between the arteries and the vein, by investigating the diffusion of solutes such as oxygen in the umbilical cord we can quantify how much solute is lost and whether this loss could affect the growth of the fetus. Firstly, we consider exchange across the cord by modelling the umbilical cord as helical vessels running inside a cylinder and solve for diffusive transport of solute within the cord tissue. We also consider the diffusion of solute along the length of the cord by building a counter-current exchange model. Our findings suggest that loss of oxygen is not significant for most cases, however shunting might become relevant for some cases characterised by abnormal cord geometry or abnormal umbilical blood flow. We can also consider exchange of other solutes such as waste products, since failure to efficiently clear these solutes could compromise the pregnancy. Keywords: mathematical biology; solute transport

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Computational Blood Flow Modelling in Health and Disease

Leszek Wierzchleyski

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Helen Wilson, Philip Pearce

In patients suffering from diseases of the blood such as malaria and sickle cell disease, red blood cells are heterogeneous and can vary in terms of stiffness and shape. It is poorly understood how this heterogeneity leads to different clinical signatures for different patients who suffer from such diseases. Through computational blood flow modelling at the cellular scale, we hope to study shed light on this problem, and thus add to a body of research concerned with personalised medicine. Keywords: Medicine, Fluid Dynamics, Computational Simulation

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Mathematical modelling of anti-adhesion therapies to tackle bacterial infections

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University of Birmingham

Sara Jabbari (University of Birmingham), Paul Roberts (University of Birmingham), Francisco Fernandez-Trillo (University of Corua)

Antimicrobial resistant bacteria is one of the biggest threats to public health today. Resistant bacteria already account for more than 750,000 global fatalities annually: a figure that could rise to upwards of 10 million individuals by the year 2050. It is critical that novel treatment strategies are developed to counteract such a hazard to human life, either to replace or be used in tandem with existing antimicrobials. Anti-virulence treatments are one such group of alternative treatments. When deployed, anti-virulence treatments prevent bacteria from utilising their arsenal of toxins. In particular we focus upon anti-adhesion therapies in which the goal is to prevent bacteria from adhering to host cells, preventing toxicity. We present an ordinary differential equation model of a theoretical anti-adhesion therapy and provide a detailed analysis of the resulting parameter space. The model will then be used to predict optimal treatment strategies with the goal to be a reduced bacterial burden.
Keywords: Antibiotic resistance, microbiology, mathematical models, anti-adhesion therapy, host-bacteria interface, ordinary differential equation model

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Identification of individual traits in collective behaviour of animal groups

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In the recent literature, much attention has been paid to the impact of individual characteristics on collective outcomes. While advances in computer vision tools have made it easier to observe, for example, collective motion, it is still challenging to identify the relevant traits of a large number of individuals. Future progress in this area could benefit immensely from developing tools that allow traits to be inferred from data that can typically be recorded at the group level. Here we propose to use the diffusion map, a convenient manifold learning technique, to infer traits from recordings of collective motion. We simulate the motion of a school of fish which heterogeneous movement traits. This simulation provides a ground truth where we know the underlying traits and the resulting trajectories. We then ask if the individual traits can be inferred from trajectory information, i.e. data that could have been captured in an actual experiment. Our results show that the diffusion map is able to identify relevant traits with good accuracy. Importantly, trait estimation is almost parameter-free and does not depend on conjectures regarding the nature of the relevant trait variables. Based on these results, it is reasonable to believe that a similar approach could be used to identify individual traits and potentially discover new trait axes directly from lab recordings available recording of animal groups. Keywords: collective dynamics, diffusion map, nonlinear manifold learning, agent-based modelling, network science, data-driven methodology

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