Applied and Computational Mathematics Seminars 2018-2019

All seminars are held at 15:10 in Room M/0.34, Senghennydd Road, Cardiff unless stated otherwise.

Programme organiser and contact: Dr Thomas Woolley

Date	Speaker	Seminar
7 May 2019	Lucy Henley & Abhishek Chakraborty	Locating bat roosts through the coupling of static acoustic detectors and motion modelling (Lucy Henley) Locating bat roosts is vital for both conservation and research purposes, as it allows biologists to study bat populations and the impact of human behaviour on populations. However, it is usually both difficult and labour intensive to find roosts using traditional search methods. I propose a novel approach for locating greater horseshoe bat roosts using data from static acoustic detectors and a mathematical model of bat movement using diffusion modelling. The model is fitted using Bayesian statistics. This method gives an actionable estimate of the roost location and narrows the search area. Modelling Calcium Signaling across a Simple Geometry (Abhishek Chakraborty) Calcium (Ca2+) signaling and its interplay with cellular mechanics plays a crucial role in development as well as in most other body processes, but it is poorly understood. In embryogenesis, malformations and cancer can result when the complex, mechanochemical

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		mechanisms go wrong. In the development of the central nervous system, cells undergo a dramatic shape change, called Apical Constriction (AC), which is essential for Neural Tube Closure (NTC). When NTC fails, the second most frequent embryo malformation, Spina Bifida, occurs. Despite its importance, AC is only partially understood. It has recently been established that tissue contractions play a crucial role and that they are driven by Ca2+. Disrupting the Ca2+ signals leads to embryo malformation, however, very few computational models of Ca2+ signalling in AC exist. The aim of my research is to develop novel, detailed computational models to fully understand AC.
2 April 2019	Zoe Ward	The cost-effectiveness of needle and syringe programmes in preventing Hepatitis C in people who inject drugs Hepatitis C virus (HCV) is a blood-borne pathogen which causes liver disease and hepatocellular carcinoma. Infections in people who inject drugs (PWID) account for over 80% of new cases each year and the prevalence of chronic HCV in this population is 45%. One of the main interventions to prevent HCV transmission is needle and syringe provision, however the cost-effectiveness of this intervention was not established in the UK or Western Europe. A systematic review of prevention benefits of needle and syringe provision (NSP) and opioid substitution therapy (OST) for HCV was undertaken and the results used in a cost-

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		effectiveness analysis for NSP. I will present these results and in addition describe allied pieces of work investigating the acceptability and cost-effectiveness of low dead space syringes which are also thought to reduce HCV transmission.
26 March 2019	Veronica Grieneisen	Cellular morphogenesis: from intracellular patterns to cell shape and tissue polarity
19 March 2019	Yulia Timofeeva	Action potential counting at giant mossy fiber presynaptic terminals: experiments and computational modelling. Neurons fire action potentials to transfer information through synaptic release of neurotransmitter. At presynaptic terminals, the pattern of action potential discharge is integrated through dynamic Ca2+ signalling by the presynaptic machinery which triggers the release of neurotransmitter. It is generally accepted that the rate and the temporal precision of action potential firing support information transfer between neurons. Here, we show that in contrast to rate and temporal coding, giant mossy fiber terminals count the number of action potentials during trains to trigger CA3 pyramidal cell firing. Our results shed light on the synaptic signal transfer mechanisms supporting an additional information coding strategy in the brain. In our study we combined electrophysiological recordings with rapid

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		presynaptic two-photon Ca2+ imaging and experimentally constrained modelling.
12 March 2019	Ian Griffiths (Mathematical Institute, University of Oxford)	iPhones and Dysons: using fluid dynamics to tailor technology As technology continues to advance, new strategies involving a range of scientific disciplines are required. Mathematicians can provide frameworks to predict operating regimes and manufacture techniques. In this talk we present two case studies: the fabrication of precision glass, for smartphones and new flexible devices; and the development of superior filters for vacuum cleaners. In each case we use asymptotic analysis to derive a model that determines the fabrication protocol required to produce a desired final product.
5 March 2019	Paul Biggs	Feature extraction, classification and visualisation in human movement analysis – a combined application of principal component analysis and Dempster-Shafer classification.
26 February 2019	Roxanna Barry	Continuum PDE models for soft tissue mechanics derived by upscaling of arrays of hyper-elastic cells Constitutive models for the deformation of soft tissues are typically constructed by fitting phenomenological models to in vitro experimental measurements. However, a significant challenge is to rationally construct macroscale models of

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		soft tissues which encode the properties of the cells and matrix which form the tissue. In this work I present a general framework to derive multiscale models for soft tissues which incorporate the properties of individual cells without assuming homogeneity or periodicity at the cell level. We consider a reduced mechanical model for an individual cell which can deform, grow and divide, and then couple these to form a network description of a one-dimensional line of cells, where each has independent material and mechanical properties. We utilise a discrete-to-continuum approach to upscale to form new (nonlinear) continuum PDE models for the tissue which allows for gradients in the cell properties, and show that these discrete and continuum formulations agree well in a variety of test problems.
19 February 2019	Dimitris Parthimo	Systems Biology from Cell to Organism We highlight the ability of mathematical tools to characterise and inform the integration of biological mechanisms operating at multiple scales, into coherent organ level responses. The cardiovascular system will provide the template for the entrainment of ionic cellular and intercellular signalling into responses manifested at the arterial wall mechanics and flow dynamics level.

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12 February 2019	Gemma Cuples	Locomotion at low Reynolds numbers Very low Reynolds number propulsion is a topic of enduring interest due to its importance in biological systems such as sperm migration in the female reproductive tract. I will talk about two different aspects of this topic, a theoretical investigation into propulsion in complex fluids and a software built to analyse sperm cell propulsion. Motivated by the fibrous nature of cervical mucus we extend Taylor's classical model of small-amplitude zero-Reynolds-number propulsion of a 'swimming sheet' via the transversely isotropic fluid model of Ericksen. In the first section of this talk I will discuss the predictions of the model for both passive and active cases, noting that the energetic costs of swimming are significantly altered by all rheological parameters and the initial fibre angle. In the second section of the talk I will introduce the work we have been doing on high-throughput computational image analysis of sperm, and the way in which the information we generate can be used in conjunction with mathematical modelling to better understand behaviour. I will discuss tracking and analysis of the flagellar waveform for a large number of cells in an automated fashion, as well as the statistical approaches we can use to achieve a simple representation of the flagellar waveform for analysis.

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5 February 2019	Josh Bull	Agent-based modelling demonstrates the impact of localised tumour cell proliferation and death on macrophage infiltration Growing tumours are infiltrated by a variety of immune cells, including macrophages, a type of immune cell which can adopt a range of pro- or anti-tumour phenotypes depending on microenvironmental cues. The spatial distribution of macrophages within a tumour varies from patient to patient and between different tumour types, and is related to patient outcome. There is considerable interest in understanding the mechanisms regulating the spatial localisation of macrophages within solid tumours and in exploiting tumour associated macrophages to deliver treatment to cancer cells. As a first step to understanding patterns of macrophage localisation within solid tumours, we consider the roles played by tumour cell proliferation and death in driving cell movement from proliferative tumour regions to hypoxic regions. This movement, induced by oxygen gradients within a tumour, must be taken into consideration when characterising patterns of macrophage infiltration. To understand the impact that this background movement has on macrophage infiltration, we first consider the infiltration of inert polystyrene microbeads into a tumour spheroid using data from. We use the CHASTE modelling framework to develop an agent-based model of microbead infiltration into a spheroid, and show how varying the rates of

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		tumour cell proliferation and death influences the patterns of bead infiltration into the tumours. Further event details.
29 January 2019 Please note new time and location. 15:10 in Room M/2.06	Gibin Powathil	Multiscale Modelling of Cancer Progression and Treatment Responses In this talk, I will present a validated hybrid individual cell-based mathematical and computational model, incorporating single-cell based intracellular dynamics, the cell microenvironment and cell-cell interactions to study the growth and progression of cancer cell mass. The model will then be used to study the effects of radiotherapy and chemotherapy. In particular, we will study the direct and indirect responses (bystander effects) of radiation therapy and further, analyse the role of cell-cycle-based tumour heterogeneity in inducing chemotherapeutic drug resistance.
23 January 2019	Katerina Kaouri (Cardiff University)	Calcium in fertilization, embyogenesis and development: modelling and experiments Calcium signalling plays a crucial role in a multitude of body processes and diseases. Furthermore, in fertilization and embryogenesis calcium signalling is strongly coupled to cellular mechanical processes. Calcium signals are complex spatiotemporal stochastic objects and mathematical modelling is a very important tool, in addition to experiments, for understanding them and making predictions. This half-day event will bring together junior and senior

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		mathematical modellers and experimentalists active in the above areas with the aim to enable networking and foster interdisciplinary collaborations. The event is supported by a “Celebrating New Appointments” grant of the London Mathematical Society (Scheme 9) awarded to Dr Katerina Kaouri (Lecturer in Applied Mathematics) and by the Cardiff University School of Mathematics. Visit the event website for more information
16 January 2019 (begins 09:30 in Room M/1.02)	Panagiota Theodoulou (COMSOL)	An extraordinary training event in COMSOL COMSOL is a piece of simulation software that can numerically solve non-linear ordinary and partial differential equations across all fields of pure and applied mathematics, physics and engineering, in 1, 2 and 3 dimensions. Specifically, across our fields of industrial and biological mathematics, Katerina and I find it to be an invaluable simulation tool. Further, it is also a perfect software suite for working with fluid flows, solid mechanics, acoustics and electrical problems. We are lucky to have Panagiota Theodoulou (from COMSOL) joining us on the 16 January, presenting a morning of training and demonstrations, thereby illustrating how the software can be used more widely by the school. The schedule is as follows:

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		09:30 Registration 09:40 COMSOL Multiphysics® Software and Application Builder 10:00 Live demo 10:45 Coffee break 11:00 Hands-on tutorial The event is completely free and open to all staff and students. However, we request that you register your interest so we can have an idea of numbers. For students, in particular, we highly recommend this opportunity as it will rapidly expand your knowledge and abilities.
4 December 2018	Andre Krause (Mathematical Institute, University of Oxford)	Some spatiotemporal phenomena in biological and physical media I will present some recent work on problems in complex spatiotemporal environments. I will first discuss diffusion-driven (Turing) instabilities in realistic flow regimes whereby interacting chemical species are advected by Stokes flow in different geometries. Such advection results in changing the regime wherein patterns emerge, as well as modulating their structure in nontrivial ways. I will spend a few minutes discussing systems of Ginzburg-Landau equations, and the role of different kinds of nonlinearities, before moving on to recent results on amplitude death due to cross-phase

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		modulation. Finally I will discuss spatiotemporal fluctuations of infection in metapopulation models of epidemics. The stochasticity in such models will be shown to be essentially negligible for small noise, leading to small fluctuations about the deterministic limit. Nevertheless, control strategies such as vaccination and treatment can be much more difficult even for such small fluctuations, and the form of the equations can lead to an effective additive noise structure which can lead to negative values of the infected proportion of the population, and hence unphysical results. Truncated noise processes can be used to recover essentially all of the qualitative features of these models while preserving non-negative populations, and non-local control strategies can ameliorate some difficulties due to the fluctuating populations. Throughout, the overall theme is on where simple canonical (e.g. linear) thinking can lead to useful understanding of the phenomena, and where such thinking can lead one astray.
27 November 2018	Neil Bezodis (Sports Science, Swansea University)	The application of mathematics to the understanding of sporting techniques and tactics: examples and future opportunities This seminar will discuss how sports science, in particular the sub-disciplines of sports biomechanics and performance analysis, have applied mathematics to aid the technical and tactical understanding of sport. Examples from recent research will be presented, mathematical challenges facing sports scientists in ongoing work will be discussed, and future opportunities

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		for mathematicians to apply their knowledge to the sporting world will be considered. Neil Bezodis is a Senior Lecturer in Biomechanics & Technology in the Applied Sports, Technology, Exercise and Medicine (A-STEM) Research Centre at Swansea University, and has worked on a range of applied biomechanics and performance analysis projects with collaborators including British Athletics and the Rugby Football Union.
20 November 2018	Vicky Brown (Faculty of Computing, Engineering and Science, University of South Wales)	Modelling Allee effects in a transgenic mosquito population during range expansion Mosquitoes are vectors for many diseases that cause significant mortality and morbidity. As mosquito populations expand their range, they may undergo mate-finding Allee effects such that their ability to successfully reproduce becomes difficult at low population density. With new technology, creating target specific gene modification may be a viable method for mosquito population control. I present a mathematical model to investigate the effects of releasing transgenic mosquitoes into newly established, low-density mosquito populations.
13 November 2018	Francois Nadal (School of Mechanical, Electrical and Manufacturing Engineering,	From a steady plume to periodic puffs during confined carbon dioxide dissolution It is now widely accepted that the continuous global warming of the atmosphere observed in the last 150 years is partially due to an increase in the atmospheric concentrations of greenhouse

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	Loughborough University)	gases, and that the storage of carbon dioxide in deep geological formations is a feasible medium term solution to the problem. The storage procedure mainly consists in injecting carbon dioxide into a brine saturated porous formation (aquifer) that is confined by an impermeable formation (cap rock). Because CO_2 is partially soluble in water, partial mixing occurs at the brine/CO_2 interface, resulting in a mixture that happens to be denser than the resident fluid. Specifically, the dissolution of the supercritical CO_2 into the brine at the CO_2/brine interface creates a heavy layer of CO_2-enriched brine, which destabilises when its thickness becomes sufficiently large. Such a gravitational instability generates convective rolls, which evolve into fingers (plumes) of CO_2-brine mixture that sink down to the bottom of the brine layer. We present here an extensive study of the stability of a single laminar plume due to gravity-induced. A topless vertical tube containing water is put in a pressure cell filled with carbon dioxide. The diffusion of CO_2 at the free surface creates a thin layer of heavy fluid underneath the surface. This unstable density gradient generates a steady laminar plume which goes downward through the entire tube. A quasi-steady flow settles in the tube, filling gradually the bottom of the tube with heavy fluid. During this laminar regime, the velocity of the plume slowly decreases due to the build-up of the background density gradient. Surprisingly, despite the decrease of the Reynolds number, the laminar plume suddenly destabilises via a varicose mode

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		into periodic pulsed puffs after an onset time which depends on the height of the tube and on the solutal Rayleigh number. This periodic regime is followed by an aperiodic regime, which lasts until the complete saturation of the solution. The observed destabilisation is explained as a result of the interplay between the feedback of the global recirculating flow and the progressive density stratification of the background fluid.
6 November 2018	Axel Almet (Mathematical Institute, University of Oxford)	Towards a morphoelastic model of a buckling intestinal crypt The intestinal epithelium exhibits remarkable rates of self-renewal to protect the small intestine and colon during digestion and injury. This monolayer is maintained by the crypts of Liehberkühn, test-tube-shaped glands that are robust in morphology and structure. While the molecular processes governing crypt morphogenesis are relatively well understood, there is a lack of understanding on the relevant biomechanical factors, especially in the context of colorectal cancer progression and injury response. In this talk, we will present our work on understanding the mechanics of crypt morphogenesis, using the framework of morphoelastic rods, which extends Kirchhoff rod theory to account for local growth. The crypt and its underlying stroma are modelled as a growing, planar rod attached to a foundation. We first discuss our analysis on the effect of spatial heterogeneity within different material properties on a simplified version of the model.

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		We then show how insights from this analysis have informed further biological specialisations, which has constituted the majority of current work.
30 October 2018	Jochen Kursawe (Faculty of Biology, Medicine and Health, University of Manchester)	Quantitative approaches to investigating epithelial morphogenesis Recent years have seen a rise in quantitative data for many biological applications. These new data can lead to challenges at each stage of the scientific method. We need to design quantitative hypotheses through mathematical models, make quantitative experimental predictions, devise methods for quantitative data analysis, and design methods for quantitative inference using models and data. My work aims to enable this quantitative transition for the integrative analysis of morphogenesis in epithelia, one of the major tissue types in animals. In this talk, I will show how I used mathematical approaches to design and analyse cell-based models of embryonic epithelia, how I use these models to make explicit experimental predictions, and how I use Bayesian techniques to compare cell-based computational models with live-imaging microscopy data.
23 October 2018	Apala Majumdar (Department of Mathematical Sciences,	The Myriad Hues of Liquid Crystals Across Mathematics, Physics and Applications Liquid crystals are classical examples of partially ordered materials intermediate between conventional solids and liquids. The concept of

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	University of Bath)	partial order is ubiquitous in nature and in this talk, we focus on nematic liquid crystals. Nematics are anisotropic liquids with no translational order and long-range orientational order, featured by the existence of special distinguished directions. We review the main continuum theories for nematic liquid crystals, the essential mathematical frameworks and how they are used to describe pattern formation in confined geometries. The pattern formation and the observable singularities arise from a complex interplay of geometry, topology, boundary effects and material properties. New analytical advances and computational techniques allow us to beautifully model pattern formation in exotic geometries, structural transitions and equally importantly, how to control structural transitions by experimental parameters to get desired properties. I will present some illustrative examples of pattern formation for nematic liquid crystals in square wells and shells emphasizing the mathematical intricacies, the underpinning physics and the plethora of novel applications in materials research in the near future.
16 October 2018	Noemi Picco (St John’s College, Mathematical Institute, University of Oxford)	Modelling Transient Traits of Cortex Evolution: the Importance of Evolving Cell Division Strategies The brain is the most complicated organ of any animal, formed and sculpted over 500 million years of evolution. The cerebral cortex is the

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		folded grey matter that forms the outside of the brain, and is the seat of higher cognitive function. Many factors influence how neurogenesis in the cortex differs between species, including the types of neurons and neural progenitor cells, the different ways in which they proliferate and differentiate, and the length of the process. Critically, to fully understand the development of the cortex we are faced with the challenge of understanding the temporal changes in cell division strategy. Combining mathematical modelling and experimental observations we incorporate these different factors to model development and evolution of the mammalian cortex. A key determinant of the neuronal production is the modulation of proliferative (self-amplifying) and differentiative (neurogenic) divisions, as well as programmed cell death. In this talk I will present models at different scales that can help us understanding how temporal changes in cell division and death events result in the final cortical size. We initially identify a developmental programme that is consistent with the temporal pattern of neuronal output in the cortex of different species. Extending this model we then investigate how the normal developmental program can take different routes, leading to pathological conditions. Finally, we ask how temporal changes in the propensity of different cell division types and cell death events unfold at the single-cell level. Throughout this talk I will

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		highlight the current limitations in the interpretation of model predictions, due to the limited data currently available, identifying a specific need for experimental quantifications. Joint work with Thomas Woolley (Cardiff University), Fernando García-Moreno (Achucarro Basque Center for Neuroscience), Zoltán Molnár (University of Oxford) and Philip Maini (University of Oxford). Funding: St John's College, Oxford.
9 October 2018	Louise Dyson (University of Warwick)	From ants to epidemiology: applications of mathematical modelling in biology and epidemiology From discovering the secrets of ant colony decisions to the modelling of treatment campaigns for eliminating endemic diseases, I am interested in the application of mathematical modelling to many different systems. In this talk I will show examples where modelling has helped to interpret and shape experimental work and data collection. I will present two case studies: understanding noise-induced bistable states in a simple model of the distribution of worker ants between two food sources; and determining if household-level contact tracing can lead to the elimination of yaws.
2 October 2018	Dr Mokarram Hossain (Zienkiewicz Centre for	Modelling curing process in polymers: From a single field to multiple fields In this talk, the modelling of curing process from a single field to multiple fields will be discussed.

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	Computational Engineering, Swansea University)	The curing of polymers is a very complex process involving a series of chemical reactions which result in the conversion of liquid low molecular weight monomer mixtures into highly cross-linked solid macromolecular structures. This phase transition from a viscous fluid to a viscoelastic solid can be modelled by a constitutive relation which is based on a temporal evolution of shear modulus and relaxation time. Some numerical examples demonstrate the capability of the model to correctly represent the evolution of elastic and inelastic material properties as well as the volume shrinkage taking place during the curing process [1]. Furthermore, in dielectric elastomers, a large actuation voltage is required to produce a desired mechanical deformation. To reduce the amount of the actuation voltage, several mechanisms can be applied and the inclusion of high dielectric permittivity fillers in the matrix material in the uncured stage is one of them [2]. Moreover, to obtain a maximum advantage from the high dielectric permittivity fillers, an electric field is applied during the curing process, which helps the particles to align in a preferred direction. In this contribution, we will show how to extend a phenomenologically-inspired large strain framework for simulating the curing process of polymers in a single field can be extended to work under the use of an electro-mechanically coupled load. The application of the proposed approach is demonstrated via some numerical examples. These illustrate that the model can predict common features in particle-filled electro-active

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		polymers undergoing curing processes in the presence of an electro-mechanically coupled load [3,4]. References [1] Hossain et al. (2009), A small-strain model to simulate the curing of thermosets, Comput., Mech., 43, 2009 [3] Romasanta et al. Increasing the performance of dielectric elastomer actuators : A review from the materials perspective, Progess in Polymer Science, 51, 188-211, 2015 [4] Hossain, M; Steinmann, P; Modelling electro-active polymers with a dispersion-type anisotropy, Smart Materials and Structures, 27(2), 2018 [4] Hossain M, Modelling the curing process with a dispersion-type anisotropy in particle-filled electro-active polymers, In review (2018)
11 September 2018	Associate Professor Amin Chabchoub (The University of Sydney)	Hydrodynamic Shock and Rogue Waves The uni-directional propagation of surface gravity water waves can be described within the framework of weakly nonlinear evolution equations such as the Korteweg-de Vries equation (KdV) in shallow-water and the nonlinear Schrödinger equation (NLS) in intermediate water depth as well as deep-water regime. Both, the KdV and NLS are physically very rich and can be for instance used to study

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		the fundamental principles of nonlinear dynamics such as the Fermi-Pasta-Ulam recurrence. Indeed, one possible explanation for the formation of ocean extreme waves, also referred to as rogue waves, is the modulation instability of nonlinear Stokes waves. This instability mechanism can be discussed within the context of exact NLS breather solutions, such as fundamental Akhmediev- or Peregrine-type breathers. A number of recent laboratory experiments on solitons and breathers in several water wave flumes will be described while novel insights on shock and rogue waves as well as domain wall physics will be discussed as well.