Applied Mathematics

Chaired by Will Graham.

Carlos Antonio Galeano Ríos: "Walking droplets: A wave-mediated non-linear non-smooth dynamical system with remarkable emergent properties."

Abstract: In 2005, Yves Couder discovered that a millimetric droplet bouncing on the free surface of a vertically oscillating bath displays a robust droplet-wave association. The droplet does not merge with the underlying bath, yielding a system that resembles a ball bouncing on a trampoline. These bouncing droplets can become unstable to lateral perturbations, impacting the bath surface at a different point each time they bounce, i.e. they start to "walk" along the surface. Each droplet impact triggers new surface waves and, in turn, the shape of the surface influences subsequent bounces. Moreover, waves are reflected of boundaries and generated by neighbouring bouncing droplets. Consequently, droplets move in response to a wave field that was created by their past trajectory and is influenced by the surrounding environment. The resulting system is formed by a collection of wave-guided wave sources, which gives rise to elaborate dynamic configurations and unique emerging properties, some of which have analogies to quantum-scale phenomena. In this talk, we will describe the key elements in the system, introduce mathematical models that capture their behaviour and conclude with an experimental demonstration.

Cameron Smith: "The auxiliary region method for coupling PDE and Brownian-based dynamics for reaction-diffusion systems."

Abstract: Reaction-diffusion systems are important tools for the study of many biological and physical phenomena, many of which span many spatial scales. Within these, there are many examples which require very detailed descriptions in some regions of space, while in the rest of the domain, large particle numbers mean that continuum methods are appropriate. For example, we could be interested in the release of calcium ions through calcium-gated channels on the endoplasmic reticulum, or want to model the formation of defects in a liquid crystal. We present the auxiliary region method - a novel spatially-coupled hybrid method which interfaces Brownianbased microscopic dynamics to the corresponding mean-field PDE through the use of "auxiliary regions" which bridge the gap between the micro and macro scales. We describe the algorithm and demonstrate its effectiveness on a large array of problems; pure diffusion, morphogen gradient formation and a travelling wave problem, spanning over one and three dimensions. We also demonstrate that the method results in small errors with no bias for particles to gravitate towards either side of the interface.

Allen Hart: "Using echo state networks to reconstruct the phase space and predict the future behavior of dynamical systems from one dimensional time series."

Abstract: We present the Echo State Network (ESN) Approximation Theorem, stating that a sufficiently large ESN trained on a 1 dimensional observation of a dynamical system can predict the next observation arbitrarily well, hence replicate the topology of a structurally stable dynamical system. We conjecture that the ESN Approximation Theorem holds for generic observation functions and call this the ESN Embedding Conjecture. The conjecture is a Takens-Theorem-like result supported by numerical evidence suggesting an ESN can find topological invariants like fixed point eigenvalues and Lyapunov exponents from a numerically integrated trajectory of the Lorenz system.

Yvonne Krumbeck: "Mortality differences suppress the number of self-incompatible mating type alleles in isogamous species."

Abstract: The study of the evolution of sexual reproduction gives rise to a number of intensely debated questions in biology. An often overlooked fact is that sexual reproduction is not always synonymous with the two sexes, male and female. Isogamous species produce sex cells of equal size, which often fall into multiple distinct self-incompatible classes, termed mating types.

A longstanding evolutionary question is what governs the number of mating types in a species? Theoretically, a rare novel type inherently has a selective advantage due to the large proportion of compatible mating partners in the population. Thus one would expect the number of mating types to grow consistently. However, this is in stark contrast with empirical observation; while some isogamous species exhibit thousands of mating types, most have only two.

In this talk, I present a mathematical analysis to quantify the expected number of mating types emerging in simple evolutionary models. We consider a situation in which mating type alleles may have diversity of mortality and model the invasion-extinction dynamics of an isogamous population. For this, we analyse two separate time scales; the short-term population dynamics and the long-term evolution when mutation events occur. Here, we use a heuristic approach to derive an analytic expression for the average number of mating types at long times. The results hold for mutants drawn from arbitrary mortality rate distributions. We predict that the number of mating types decreases with the rate of sexual reproduction, and is lowered further as the variance of mortality increases. Our analytic results are consistent with existing empirical data and thus provide a potential resolution to this longstanding question.

Statistics

Chaired by Lizzi Pitt.

Dr Tim Paulden: "Become a SCAM artist! State-of-the-art modelling in one line of R." Abstract: In this talk, Dr Tim Paulden will introduce the classic tennis modelling challenge of converting world rankings into win probabilities, and demonstrate that a relatively new technique called SCAM (shape-constrained additive modelling) can "automatically" generate competitive predictions that respect the problem's monotonicity constraints. Several higher-level modelling concepts will also be discussed, including effective methods of model assessment and the perils of overfitting. The talk will begin from first principles – no previous knowledge of modelling is assumed!

Tom Smith: "" Abstract:

Nadeen Khaleel: "Bayesian Inference for Crime Incidence in the USA."

Abstract: Presence of crime is a constant in cities, however, the relationship between locations of crime incidences and social and economic factors can vary between cities. Modelling crime locations as a point pattern with log-Gaussian Cox process allows us to understand the impact of such factors and the spatial dependency structure within cities but is impeded by sparse and unreliable data. Here we consider algorithms for inference for log-Gaussian Cox processes for more complex models to account for data sparsity and measurement error. We build on an algorithm from Gómez-Rubio & Rue (2018) that combines the flexibility of MCMC and the efficiency of integrated nested Laplace approximations. We can implement this algorithm to perform inference for point patterns across disjoint regions, such as cities that do not share a boundary, and to pool data between these regions to provide more confidence in our inference without a drastic

penalty on computation time.

Robbie Peck: "Optimal Decisions in the Portfolio Problem."

Abstract: Suppose a company has a portfolio of various drugs in development which if successful will become available for large phase III trials in the near future. We consider the portfolio problem, which deals the optimal allocation of a 'Research and Development' budget to phase III confirmatory trials within some planning horizon. We require a design strategy to allocate the overall budget to the available drugs for phase III trials, in order to maximise the expected net present value of the portfolio. This design strategy must specify the optimal phase III sample sizes, given the remaining budget and drug parameters.

Previous approaches to this problem have used integer programming formulations or simulation models. We use a dynamic programming approach to derive the optimal decisions, which may scale up more efficiently in computational workload as the portfolio considered becomes more complex.

The use of group sequential designs which allow early stopping can benefit the portfolio by increasing the time one can market the drug until patent expiry, in addition to allowing the reinvestment of saved resources back into the portfolio. We can consider the value group sequential methods bring to a portfolio within this framework.

Lightning Talks

Chaired by Jack Betteridge.

Cohort 5 will each have 3 minutes to present the research they will be undertaking over the summer, or research they have done at an ITT.

Simone Appella: "Semi-Implicit Semi-Lagrangian (SISL) Scheme for Shallow-Water Equations"

Oluwatosin Babasola: ""

Thomas Bartos: ""

Tom Davies: ""

Margaret Duff: ""

Marco Murtinu: ""

Laura Oporto Lisboa: ""

Eileen Russell: ""

Zsófia Talyigas: ""

Jordan Taylor: ""

Jason Wood: ""

Josh Young: ""

Probability

Chaired by Trishen Gunaratnam.

Tyler Helmuth: "Approximate sampling algorithms in statistical mechanics."

Abstract: Sampling from high-dimensional probability distributions is an important task. A simple example of this task is to sample a random independent set of a graph. I'll use this example, known in statistical mechanics terminology as the hard-core model, to introduce and discuss efficient approximate sampling algorithms. In particular I will describe the existence of a computational phase transition for this problem, as well as some recent progress on approximate sampling in the dense phase.

Tom Finn: "A New Phase of Coexistence in Random Competition Models." Abstract: Start two random growth processes at distinct vertices in \mathbb{Z}^d at rate 1 and rate λ , for $d \geq 2$. We say that both processes coexist if one does not encapsulate the other in finite time. This is known as the two-type Richardson model and it remains an open conjecture to prove that coexistence occurs with positive probability if and only if $\lambda = 1$. The reason that these random competition models are so difficult to analyse is that they lack many pleasant properties, such as monotonicity, that makes such proving such results extremely challenging and new methodologies are required.

In this talk we discuss another random competition model called first passage percolation in a hostile environment (FPPHE), in which one random growth process is inhibited by randomly encountering and activating another growth process. We shall explore the behaviour of such a model and see that it does observe a coexistence phase in multiple scenarios.

Kevin Olding: "Optimal high frequency market making strategies."

Abstract: Market makers are dealers in financial markets who create liquidity by quoting prices at which they are willing to buy and sell an asset. Market makers profit by offering to sell at higher prices than those at which they will buy, but may face losses due to adverse price movements in the underlying asset when they hold inventory, and also when trading with agents with superior information about the future price of the asset.

Whilst traditionally the role of the market maker was played by large investment banks, in practice any agent may become a market maker by placing limit orders into the limit order book. In particular, in modern markets such strategies are often employed by high frequency traders seeking to profit from market making strategies.

In this talk we will consider what such optimal market making strategies might look like for high frequency traders, with a particular focus on the model proposed by Avellaneda and Stoikov (2008).

Paolo Grazieschi: "Convergence of the three-dimensional Ising-Kac model to ϕ_3^4 "

Abstract: We will introduce the Ising model and then change the way particles behave by introducing a long range interaction. The resulting system, called Ising-Kac model, is studied in its scaling properties and ultimately the goal is to prove that a suitably rescaled version of it converges to the ϕ_3^4 equation. We will also discuss the regularity difficulties that this equation poses and how to define a concept of solution.

Research Motivated by Industrial Problems

Chaired by Tom Finn.

Adwaye Rambojun: "A hybrid approach to finding bones of the hand."

Abstract: In this talk, we will demonstrate how to merge a shape model with a texture model. We then use the hybridisation to perform bone segmentation. Particular emphasis will be laid on different Neural Network architectures that can be used for shape modelling. We will also address the problem of initialising shape models onto a new image and how this affects the end result.

Kate Powers: "Modelling Surge in Turbocharger Compressors."

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

In this talk, I will describe a new modelling approach for surge that was developed from compressible, rotating, Navier-Stokes equations. I will discuss the motivation behind developing a new approach, share insights into the surge phenomenon that our model has given us, and provide validation through comparison to experimental data.

Daniel Burrows: "On-line drill system parameter estimation and hazardous event detection." Abstract: Oil welling operations involve drilling methods that are susceptible to events that compromise efficiency and, in extreme cases, lead to hazardous outcomes. One such event is called washout, in which drill fluid bypasses the motor by flowing through a hole in the wall of the drill pipe, leading to a reduction in the pressure applied to the drill motor.

Modelling the evolution of the state of washout as a Markov process, we use the available information in the form of noisy measurements collected on the surface to construct a hidden Markov model that relates the measurements to the state of the washout. We then explore the application of sequential Monte Carlo methods (SMC) to this model to provide an on-line hazard detection framework.

Numerical Analysis

Chaired by Shaunagh Downing.

Catherine Powell: "Surrogate-accelerated Bayesian inversion for the determination of the thermal conductivity of a material."

Abstract: Determining the thermal properties of a material is an important task in many scientific and engineering applications. Indeed, how a material behaves when subjected to high or fluctuating temperatures can be critical to the safety and longevity of a system's essential components. The laser flash experiment is a well-established technique for indirectly measuring the thermal diffusivity of a material. In a controlled experiment, a laser is fired at a sample of the material from below, and the temperature is measured on the opposite surface over a period of time.

In this talk, we pose the problem of determining the thermal conductivity of a material, using temperature data obtained via the laser flash experiment, as a Bayesian inverse problem. The laser intensity is also treated as uncertain. Adopting a Bayesian approach allows for prior beliefs about uncertain model inputs to be conditioned on experimental data to determine a posterior distribution, but probing this distribution using sampling techniques such as Markov chain Monte Carlo (MCMC) methods can be incredibly computationally intensive (or simply infeasible). This is especially true for forward models consisting of time-dependent partial differential equations (as in the laser flash experiment).

To accelerate MCMC sampling, we introduce a parametric surrogate model that takes the form of a stochastic Galerkin finite element approximation and show how it can be used to sample efficiently from an approximate posterior distribution. This approach gives access not only to the sought-after estimate of the thermal conductivity, and hence, diffusivity, but also important information for uncertainty quantification. Computational savings of orders of magnitude are achieved over standard MCMC sampling.

This is joint work with James Rynn and Simon Cotter from the University of Manchester and Louise Wright from the National Physical Laboratory (NPL).

Owen Pembery: "Nearby preconditioning for the Helmholtz equation, with application to uncertainty quantification."

Abstract: The simplest PDE modelling propagating waves is the Helmholtz equation, a deceptivelysimple-looking second-order elliptic PDE.

If we discretise the Helmholtz equation via the finite-element method, we then need to solve linear systems that are (for high-frequency waves) large, non-Hermitian, and indefinite. In general, solving these linear systems is very difficult. Therefore, we precondition our linear systems (we multiply them with a suitably-chosen matrix - a preconditioner) to make them easier to solve.

However, if we are modelling waves moving in random media, we need to perform Uncertainty Quantification (UQ). That is, we solve lots (thousands) of these linear systems, corresponding to lots (thousands) of realisations of our random media. Therefore, on the face of it, we need to construct lots (thousands) of different preconditioners. Constructing all these preconditioners may be very computationally expensive. To try and reduce this expense, we investigate how well a preconditioner for one realisation of the Helmholtz equation works as a preconditioner for a different realisation. (So that we can re-use our preconditioners many times.)

We prove that if the two realisations are nearby, then a preconditioner for one realisation works well for the other realisation (for precise meanings of 'nearby' and 'works well'). We also apply this technique to a UQ algorithm for the Helmholtz equation, and see from computational results that we get significant speedup across a range of frequencies.

Jack Betteridge: "Efficient solvers for semi-implicit hybridised DG methods in fluid dynamics."

Abstract: For problems in Numerical Weather Prediction (NWP), time to solution is a critical factor. Semi-implicit time-stepping methods can speed up geophysical fluid dynamics simulations by taking larger time-steps than explicit methods. This is possible because they treat the fast (but physically less important) waves implicitly, and the time-step size is not restricted by the CFL condition for these waves. One disadvantage of this method is that an expensive linear solve must be performed at every time step, however, using an effective preconditioner for an iterative

method significantly reduces the computational cost of this solve, making a semi-implicit scheme faster overall.

Higher-order Discontinuous Galerkin (DG) methods are known for having high arithmetic intensity making them well suited for modern HPC hardware, but are difficult to precondition due to the large number of coupled degrees of freedom. This coupling arises since the numerical flux introduces off diagonal artificial diffusion terms. By using a hybridised DG method we can eliminate the original coupling and instead couple the equations to a smaller global system on the trace space, which is easier to precondition. This is achieved by considering the numerical flux variables which only lie on the facets of the mesh. We build on recent work[1] in this area by solving the resultant system using a non-nested geometric multigrid technique instead[2].

We discretise and solve the non-linear shallow water equations, an important model system in geophysical fluid dynamics, and demonstrate the effectiveness of the multigrid preconditioner for a semi-implicit IMEX time-stepper. The method is implemented in the SLATE language, which is part of the Firedrake project. Firedrake is a Python framework for solving finite element problems via code generation.

This is joint work with Thomas Gibson (Imperial), Ivan Graham (Bath), Lawrence Mitchell (Durham), Eike Müller (Bath).

[1] Kang, Shinhoo and Giraldo, Francis X and Bui-Thanh, Tan. IMEX HDG-DG: a coupled implicit hybridized discontinuous Galerkin (HDG) and explicit discontinuous Galerkin (DG) approach for shallow water systems arXiv preprint arXiv:1711.02751, 2017

[2] Cockburn, Bernardo and Dubois, Olivier and Gopalakrishnan, Jay and Tan, Shuguang. Multigrid for an HDG method IMA Journal of Numerical Analysis 34(4):1386–1425, 2014

Hayley Wragg: "Modeling high frequency electromagnetic propagation – A generalised raylaunching approach."

Abstract: Wireless communication has become a significant part of society with recent developments to the internet of things increasing the number of devices connecting in one home. This has increased user demand for bandwidth and lead to developments in new transmitter types. One of these developments is ultra-high frequency transmitters.

In this talk I will look at ray-launching methods for modeling the propagation of these devices in cluttered unknown environments. The adapted ray-launching approach I will present speeds up the optimisation process and conserves information which may be used for sensitivity analysis.