Applied Mathematics MSc Projects 2019 -2020
Imperial College London

Vortex dynamics using network-based modelling

Dr. Peter Baddoo & Prof. Darren Crowdy

This project uses a novel combination of analytic and data-driven tools to understand two-dimensional turbulence. In particular, we are interested in elucidating the fundamental physical mechanisms associated with vortical interactions with solid boundaries [1]. The project will begin by deriving closed form solutions for the trajectories of a point vortex embedded in a potential flow within a periodic domain [2]. Whilst the solution is likely to be straightforward for a single vortex, it is expected that the problem will become analytically intractable for large numbers of vortices as the inter-vortex relationships become prohibitively complicated. However, recent advances in network science have opened new avenues for analysing interactions among a large group of connected elements. Accordingly, we will develop a network-theoretic approach to understand the behaviours and trajectories of large groups of vortices and their interactions with solid boundaries; previous work in this vein [3] has not considered the effects of boundaries, which have been known to dominate the behaviour.

This project is relevant to students with interests in fluid mechanics, complex analysis, and network science.

Learning outcomes:

1. Modelling of turbulence using potential flow theory
2. Use of periodic conformal maps, possibly between multiply connected domains
3. Competency with using networks to model large-scale interactions between vortices.

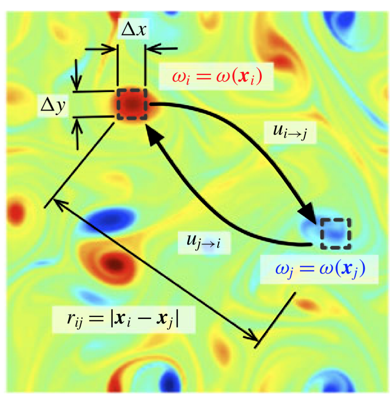


Figure 1: The vortex network model considered in [3]. The MSc project will extend the model to consider the effects of solid boundaries.

References

[1] P. G. Saffman. *Vortex Dynamics*. Cambridge University Press, Cambridge, 1993.

[2] P. J. Baddoo and D. G. Crowdy. Periodic Schwarz–Christoffel mappings with multiple boundaries per period. *Proc. R. Soc. A Math. Phys. Eng. Sci.*, 475(2228), 2019.

[3] K. Taira, A. G. Nair, and S. L. Brunton. Network structure of two-dimensional decaying isotropic turbulence. *J. Fluid Mech.*, 795:R2, 2016.

Can superfluids rotate rigidly? – Dr Ryan Barnett

A superfluid is a substance that flows with zero viscosity. When mechanically rotated (e.g. when in a spinning bucket) superfluids typically will form a vortex lattice, in stark contrast to classical fluids. This is because the velocity of a superfluid is the gradient of a phase having quantum mechanical origins: $\mathbf{v} = \frac{\hbar}{m}\nabla\theta$. As a result, the voticity, $\nabla \times \mathbf{v}$, is zero everywhere except the positions marking the vortex centres (where the phase is ill-defined). Rigid rotation – where $\nabla \times \mathbf{v}$ is a non-zero constant everywhere – clearly cannot be obtained for this case.

The above does not apply when the atoms forming the superfluid have internal spin degrees of freedom. For this case, the vorticity is related to the spin direction, denoted by unit vector $\mathbf{n}$, as

$$\partial_x v_y - \partial_y v_x = \frac{\hbar}{2m}\mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n})$$

(restricting to two spatial dimensions for simplicity). This elegant and geometric equation is known as the Mermin-Ho relation.

The aim of this project is to investigate if spinor fluids can rotate in ways similar to their classical counterpart. That is, can such steady state solutions be found in the rotating frame of reference? A recent affirmative result along these lines was obtained in [1]. Spinor superfluids with spin-orbit coupling – a topic of considerable recent experimental progress – is likely a crucial ingredient and will be investigated in this context.

[1] Sandro Stringari, *Diffused Vorticity and Moment of Inertia of a Spin-Orbit Coupled Bose-Einstein Condensate* Phys. Rev. Lett. 118, 145302 (2017)

The four-dimensional quantum Hall effect – Dr Ryan Barnett

Quantum Hall states have become paradigmatic condensed matter systems exhibiting the interplay between topology and physics [1]. The understanding of such systems starts with a quantum mechanical textbook exercise: finding the energy levels of an electron confined to two spatial dimensions under the presence of a perpendicular magnetic field. Such systems have topologically protected boundary modes, due to a deep principle known as the bulk-boundary correspondence. The behavior of such systems can be quantified by a topological invariant called the first Chern number. Recently, in cold-atom and photonic systems, a four-dimensional version of the quantum Hall effect has been achieved (here time plays the role of the fourth dimension) [2,3].

After becoming familiarised with the quantum Hall effect, this project will explore this new area – 4d quantum Hall systems. In particular we will seek a generalisation of the Haldane model to 4d systems.

[1] J Avron and D Osadchy, *A Topological Look at the Quantum Hall Effect* Physics Today 56, 8, 38 (2003)

[2] M. Lohse *et al.*, *Exploring 4D quantum Hall physics with a 2D topological charge pump*, Nature 553, 55 (2018)

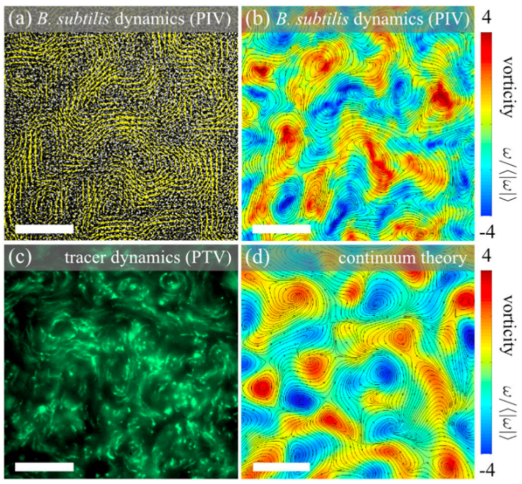
Project: "Generation of mean flows by locally forced Rossby waves".
Supervisors: Michael Haigh and Pavel Berloff

This Project is ideal for a student with strong interest in fluid dynamics and aiming to develop both theoretical and numerical modelling skills.
There are solid preliminary results that ensure a publication coming out of this project, provided investment of substantial but straightforward efforts.

This problem is geophysically motivated by the need to understand the role of mesoscale eddies (i.e., oceanic weather) in maintaining fast eastward jet currents and their westward recirculations.
The aim of the Project is to use an idealised rotating shallow-water model to explore the fundamental aspects of mean-flow generation by localised forcing in the ocean.
In the idealised setup, the localised forcing excites Rossby waves that exist, due to the combined effect of the Earth sphericity and rotation, and once excited propagate away in all directions.
This propagation drives zonal momentum fluxes to converge on the waves' source, thus, driving an eastward mean flow.
The quantitative behaviour of this process strongly depends on the physical parameters of the system, owing to the related dependences of the Rossby waves.
This problem has previously been considered in the single-layer shallow-water system (Haigh and Berloff 2018, 2019), as well as in the quasigeostrophic approximation.
This MSc project will involve an exploration of essential parameters (e.g., background flow, stratification, forcing properties), in the two- and/or three-layer shallow-water approximations.

Dynamics of Active Fluids: an analytical and numerical exploration of the Toner-Tu equation
Dr. T. Bertrand

Active systems take energy from their environment to transform it into motion. These systems are driven far from equilibrium [1] and display a wealth of new phenomena forbidden by equilibrium thermodynamics, including the emergence of novel collective properties including large scale collective motion [2], clustering [3], and self-jamming [4]. Studying active matter offers hope to uncover new physics, shine light on complex biological processes and perspectives to develop functional materials and smart devices. Complex and robust collective behaviors can be the result of interactions between very simple constituent agents; finding a general framework to understand how active particles synergistically interact to perform a task is appealing and has many applications.



Example of active fluid dynamics: bacterial turbulence, reproduced from [12].

While the dynamics of conventional fluids is governed by the famous Navier-Stokes equation [5], the dynamics of active fluids is well-described by the Toner-Tu equation [6,7,8,9,10]. This equation was originally derived on the basis of symmetry considerations [6]. For the past two decades, several studies have rederived hydrodynamic equations by systematically coarse-graining microscopic models of active particles to finally end up with a Toner-Tu equation [10].

Using a combination of analytics and numerical simulations, we will study the emergent phases stemming from the activity in the Toner-Tu equation. On the numerical side, we will develop methods to numerically solve the Toner-Tu equation for a variety of parameters. In a first step, we will base our methods on classical pseudo-spectral and spectral methods which were hugely successful in classical hydrodynamics [11].

Learning outcomes:
-The project provides the interested student an occasion for both analytical and computational work;
-The analytical part of the project will involve analysis of partial differential equations, linear stability analysis;
-The computational part of the project will involve developing new numerical methods for PDEs (based on our knowledge of techniques to solve hydrodynamic equations to explore the phase diagram of this model numerically;
-The results of this project are expected to lead to a publication.

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[2] A. Bricard, J-B Caussin, N. Desreumaux, O. Dauchot, and D. Bartolo. Nature, 503(7474):95–98, 2013.
[3] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck. Phys. Rev. Lett., 110:238301, 2013.
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Computational models of cellular tissues
Dr. T. Bertrand

D'Arcy Thomson published in 1917 a treatise "On Growth and Form" in which he suggested that morphogenesis could be explained by forces and motion. For a while this idea took a backseat in favor of genetics and chemical communication within cell assemblies, but it was recently revisited and it was suggested that mechanical forces play an important role in the organization and function of living tissues [1]. The importance of mechanics in collective migration is well accepted; however, a lot of contradicting evidence has emerged. The interplay between cell-cell and cell-substrate interactions is key to collective cell migration, and is often deregulated during pathologies.

Most of the theoretical effort to understand single cell dynamics relies on simplistic models of stochastic motion, where cell motion is described as a simple or persistent random walk, Lévy walk or composite processes such as intermittent random walks [2]. A recent study revealed a universal coupling between cell speed and cell persistence [3] despite the multiplicity of migration patterns of different eukaryotic cell types. Further, it was observed that as the density of cells increases, cells become confluent, cell dynamics slows down and the cell monolayer displays a rich glassy behavior [4]. Using a vertex model [5] for confluent tissues, it was shown that a rigidity transition exists for confluent tissues. This rigidity transition has for control parameters single-cell properties such as adhesion and cortical tension [6]. How do these collections of active particles (the cells) behave at very high density (e.g. dense confluent tissues)? What are their mechanical properties? These are open questions. Much effort has been devoted to understanding passive thermal and athermal particulate matter [7]. These systems generically go through a rigidity transition from a liquid-like state at low density or high temperature to a solid-like state at high density or low temperature. Jamming is an emergent concept in biophysics [8]. Does active matter (like tissues) also generically display jamming/glassy like features?

Using theoretical modelling and numerical simulations, the goal of this project is to understand the intimate link between the macroscopic response of complex biological materials and the microscopic details of their dynamics and intricate interactions. In particular, by studying the mechanical properties of cells and tissues in silico, we hope to shine light on the mechanisms behind collective remodeling of biological tissues. We will develop and compare multiple computational models of tissue dynamics. First, we will generalize the Vertex model to encompass the physical model of cell persistence introduced in [3]. Secondly, we will develop dedicated soft deformable particles simulations [9,10] incorporating direct control parameters such as cell density, cell pressure and cortical tension. These simulations will allow us to study the effect of activity and elasticity/deformability of the cells. Simulations of deformable particles will allow us to do this as a function of density.

Learning outcomes:
-The project provides the interested student with an experience in the field of biomathematics;
-The project relies on the development of multiple computational models, so offers a variety of opportunities to expand the skillset of the interested student;
-Experimental data may be available to compare with theoretical predictions;
-The results of this project are expected to lead to a publication.

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[8] M. Sadati, N. T. Qazvini, R. Krishnan, C. Y. Park, and J. J. Fredberg. Differentiation , 86(3):121 – 125, 2013.
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Dynamics of dense suspensions of mechanosensitive organisms
Dr. T. Bertrand

Active systems take energy from their environment to transform it into motion. These systems are driven far from equilibrium [1] and display a wealth of new phenomena forbidden by equilibrium thermodynamics, including the emergence of novel collective properties. Studying active matter offers hope to uncover new physics, shine light on complex biological processes and perspectives to develop functional materials and smart devices. Complex and robust collective behaviors can be the result of interactions between very simple constituent agents; finding a general framework to understand how active particles synergistically interact to perform a task is appealing and has many applications. It is in general only through their interactions with other particles and the environment that active particles display non-equilibrium features and are distinguished from their passive counterpart; these can have spectacular consequences. For instance, dense suspensions of interacting active particles can display large scale collective motion [2], clustering [3], and self-jamming [4].

To apprehend their immediate environment and position themselves in space, most living organisms use a combination of vision and hearing but also sensing of internal and external mechanical strains applied to their body. Even very simple organisms utilize mechanosensing to explore their surroundings, usually by contact. In particular, we are interested here in the paramecium, a motile unicellular eukaryotic micro-organism, living in stagnating waters. It feeds on bacteria and is capable of detecting the presence of obstacles on its path. When the anterior part of its body touches an obstacle, the paramecia swim backward for a brief instant, before resuming its progress forward in a new direction of motion. This is called the avoidance reaction. When the posterior part of its body come in contact with a mechanical stimulus, the paramecia tries to escape by increasing its swimming speed, thus accelerating its motion in the same direction [5].

Using a combination of analytics and numerical simulations, we will study the dynamics of dense assemblies of mechanosensitive organisms. In order to do this, we will use lattice Monte Carlo simulations on a lattice [6] and we will also develop a model of active Brownian particles in continuous space and time. We will compare the results of those simulations to analytical results we will obtain using kinetic theory.

Learning outcomes:
-The project provides the interested student an occasion for both analytical and computational work;
-The analytical part of the project will involve random walks theory, lattice models in statistical mechanics, and kinetic theory;
-The computational part of the project will involve both Monte Carlo techniques on lattice as well as numerical methods for active Brownian Dynamics;
-The supervisor has an ongoing collaboration with experimentalists, as such experimental data may be available to compare with theoretical predictions;
-The results of this project are expected to lead to a publication.

[1] M. E. Cates. Reports on Progress in Physics, 75(4):042601, 2012.
[2] A. Bricard, J-B Caussin, N. Desreumaux, O. Dauchot, and D. Bartolo. Nature, 503(7474):95–98, 2013.
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Phase Transitions in Models of Opinion Formation
Dr. T. Bertrand

The emergence of complex behavior in a system of interacting agents or particles is one of the most fascinating problems. Examples can be found in any field of science, from the collective migration in cellular tissues to swarming in schools of fishes and flocks of birds, and pattern formation in chemical and physical systems. At all scales, understanding the intimate link between the macroscopic properties of the system and the detail of the interactions at the microscopic scale is one of the major challenge in complex systems.

More recently, applied mathematicians and physicists have ventured in the field of social sciences and attempted to model the behavior of social groups. The formation of public opinion is among these challenging problems. It reveals a complex dynamics which can be influenced by a variety of internal and external sources such as mass media and social networks, extremists groups, charismatic political leaders etc.

The goal of this project is to build upon previous studies which have used models based on active Brownian particles to model collective opinion formation and understand the emergence of consensus. In physical terms, this system can be regarded as a model of phase transitions in large assemblies of interacting agents. This project entails generalizing a model of interacting active Brownian agents which will be studied by means of agents-based simulations. Simultaneously, we will coarse-grain this model to study it at the level of the associated Fokker-Planck equation. Our goal will be to study and control the onset of phase transitions (such as consensus or opinion segregation) for instance in systems with followers and leaders, systems where we included a fraction of extremists etc.

Learning outcomes:
-The project provides the interested student with an experience in the techniques of statistical mechanics applied to social sciences;
-The project will combine both analytics and the development of numerical simulations;
-The results of this project are expected to lead to a publication.

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[3] J. Garnier, G. Papanicolaou and T-W. Yang, Vietnam J. Math. 45:51-75 (2017)
[4] J. Garnier, G. Papanicolaou and T-W. Yang, Discrete and Continuous Dynamical Systems Series B 24(2)851-879 (2019)

Michele Coti Zelati: Enhanced diffusion and hypocoercivity

The goal of this project is to study the enhanced diffusion properties of a passive scalar f that satisfies the advection diffusion equation

$$\partial_t f + \boldsymbol{u} \cdot \nabla f = \nu \Delta f, \tag{1}$$

or the vector equation for the passive vector B

$$\partial_t B + (\boldsymbol{u} \cdot \nabla) B = (\nabla \cdot B)\boldsymbol{u} + \nu \Delta B, \tag{2}$$

where $\nu > 0$ is a small diffusion parameter and $\boldsymbol{u}$ is a given, time-independent and divergence-free velocity vector field. In fairly general settings, it is not hard to show that the energy of the solution (namely, the L^2-norm) decays exponentially as $\mathrm{e}^{-\nu t}$. However, it is expected that the presence of the flow $\boldsymbol{u}$ speeds up the rate to $\mathrm{e}^{-\nu^q t}$, for some $q \in (0, 1)$ depending on $\boldsymbol{u}$. This is a manifestation of a phenomenon called *enhanced diffusion*, and it has been proven with optimal rates only in the case when $\boldsymbol{u} = (u(y), 0)$ is a shear flow with a finite number of critical points [**1**]. The goal of this project is to employ an energy method called *hypocoercivity* [**2**], which allows to study finer properties of the flows by looking at commutators between the transport and the diffusion terms. Several settings are physically relevant and interesting:
◇ In a 3D periodic domain, with $\boldsymbol{u} = (u(y), 0, 0)$, or $\boldsymbol{u} = (u(y, z), 0, 0)$, or various "shear" versions of this.
◇ In a 3D cylindrical domain of the type $\mathbb{T} \times D$, where $\boldsymbol{u}$ is a pipe flow, namely $\boldsymbol{u} = (1 - y^2 - z^2, 0, 0)$.
The goal is to describe in mathematically rigorous terms the features of Figure 1 and similar

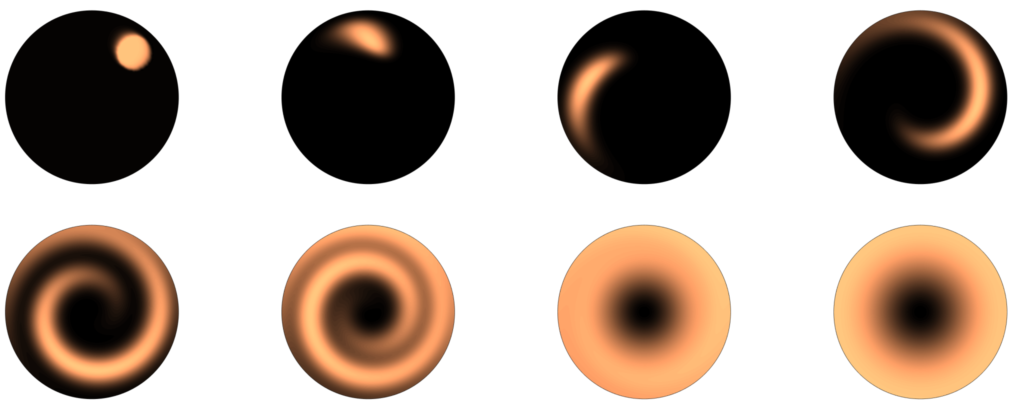

FIGURE 1. The evolution of a drop of slightly diffusive "cream" radial stirred into a "cup of coffee" with impermeable walls. Initially, pure advection is the dominant effect. As time progresses, the solution becomes radially symmetric. After this time, the cream simply diffuses across the (circular) streamlines.

Prerequisites. Student taking on this project is required to have some basic understanding of differential equations, multivariable calculus, Fourier series and Hilbert spaces.

References

[1] J. Bedrossian and M. Coti Zelati, *Enhanced dissipation, hypoellipticity, and anomalous small noise inviscid limits in shear flows*, Arch. Ration. Mech. Anal. **224** (2017), no. 3, 1161–1204.

[2] C. Villani, *Hypocoercivity*, Mem. Amer. Math. Soc. **202** (2009), no. 950, iv+141.

Michele Coti Zelati: Mixing by random flows

We want to understand the stochastic flow $\phi^t : \mathbb{T}^d \to \mathbb{T}^d$, $t \geq 0$, defined on $\mathbb{T}^d = [0, 2\pi)^d$ by the random ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi^t(x) = u_t(\phi^t(x)) + \sqrt{2\kappa}\,\dot{W}_t, \qquad \phi^0(x) = x, \tag{1}$$

where $\kappa \in [0, 1]$ and the random velocity field $u_t : \mathbb{T}^d \to \mathbb{R}^d$ is divergence-free. The question is how to construct flows which possess a strictly positive Lyapunov exponent: that is, for which there exists a constant $\lambda > 0$ such that for every $x \in \mathbb{T}^d$ we have that

$$\lim_{t\to\infty} \frac{1}{t} \log |D_x\phi^t| = \lambda > 0, \qquad \text{with probability } 1. \tag{2}$$

Here, $D_x\phi^t$ refers to the Jacobian matrix of ϕ^t taken at x. For this, we will need to become familiar with a bunch of concepts from random dynamics. It is well-known that (1) is closely related to the passive scalar equation

$$\partial_t g_t + \boldsymbol{u} \cdot \nabla g_t = \kappa \Delta g_t, \qquad g_0 = g, \tag{3}$$

via the formula $g_t = \mathbf{E} g \circ (\phi^t)^{-1}$, where there is no need of $\mathbf{E}$ if $\kappa = 0$. In the cases studied in [**1**, **2**], the consequences of (2) are that for any g,

$$(\kappa \in [0, 1]) \qquad \|g_t\|_{H^{-1}} \leq D\mathrm{e}^{-\gamma t}\|g\|_{H^1}, \tag{4}$$

$$(\kappa > 0) \qquad \|g_t\|_{L^2} \leq \frac{D}{\kappa}\mathrm{e}^{-\gamma t}\|g\|_{L^2}, \tag{5}$$

for all $t > 0$, for some deterministic $\gamma > 0$ and some random constant D independent of κ. These results are very interesting, as they quantify precisely a transfer of energy of g to high frequencies, or equivalently the creation of small scales, which is at the heart of turbulence theory (Figure 1).

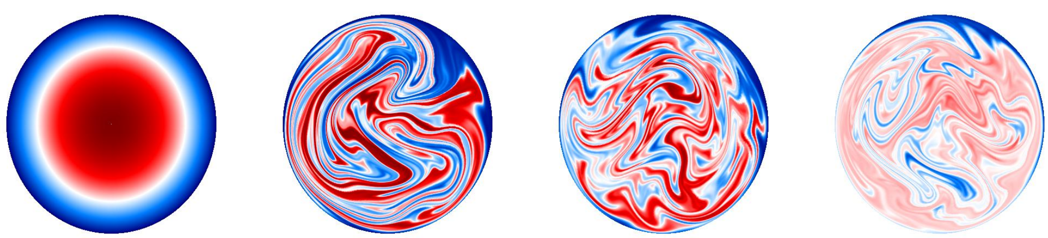

FIGURE 1. The high (red) and low (blue) concentrations of a scalar in a disc when stirred by a random flow. At the beginning, stirring is dominant and small scales are created, while later diffusion is dominant, and the main visual effect is blurring (pictures by J. Vanneste, Edinburgh).

Prerequisites. Student taking on this project is required to have some basic understanding of stochastic differential equations, multivariable calculus, Fourier series and Hilbert spaces.

References

[1] J. Bedrossian, A. Blumenthal, and S. Punshon-Smith, *Almost-sure enhanced dissipation and uniform-in-diffusivity exponential mixing for advection-diffusion by stochastic Navier-Stokes*, arXiv e-prints (Nov. 2019), available at 1911.01561.

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Project 1: Reduced models of the Madden-Julian Oscillation

Professor Colin Cotter

The Madden-Julian Oscillation (MJO) is a mode of oscillation of the Earth's atmosphere, with each cycle lasting 30-60 days. It has a strong effect on the Indian and West AFrican summer monsoon, and so predicting the MJO behaviour better would have critical impact on the livelihoods of farmers and the general population of people living in those areas.

In this project, we will investigate a simplified model of the MJO mechanism proposed in Majda and Stechman (2009). This model is an approximation of the full equations of motion of the atmosphere, the simplest form of which has everything linearised except for a nonlinear term representing convection. We will develop a finite element method for these equations based on the compatible finite element framework developed in Cotter, Natale and Shipton (2016), and then implement it using the Firedrake code generation system (`firedrake-project.org`). We will investigate reductions of the full 3D equations where the vertical structure is restricted to be polynomials of some low degree, enabling the model to be run on a regular laptop or workstation, and explore the behaviour of the solution with the polynomial degree.

For more information on the Majda and Stechman model see the Springer Brief textbook "Tropical Intraseasonal Variability and the Stochastic Skeleton Method" which is available as an e-book from the college library.

This project will enable the student to learn something about the MJO and its dynamics, together with state-of-the-art numerical methods being used for numerical weather prediction.

Project 2: The pressure-robust CR1-DG0 scheme for the rotating shallow water equations

Professor Colin Cotter

The compatible finite element method was proposed for geophysical fluid dynamics in Cotter and Shipton (2012) and now underpins the Met Office dynamical core (the fluid dynamics part of an atmosphere model) for their new modelling system that is scheduled for operational use in the mid 2020s. Compatible finite element methods preserve the fundamental vector calculus identities $\nabla \cdot \nabla \times = 0$ and $\nabla \times \nabla = 0$ at the discrete level, which translate to important wave propagation properties of the finite element method that make the discretisation work. One disadvantage of the method is the presence of nondiagonal "mass matrices" that mean that matrix-vector systems must be solved even when explicit time integration methods are used. On the other hand, the CR1-DG0 finite element method has diagonal mass matrices, so explicit timestepping can be easily made to run very fast. However, it lacks the discrete vector calculus identities of compatible finite element spaces. Recently, it was shown that the CR1-DG0 method can be made more pressure robust by applying a local projection operator to various terms in the equation. This has been explored in the context of Navier-Stokes equations but not in the rotating compressible systems of numerical weather prediction. In this project we will explore the pressure robust version of the CR1-DG0 method for the linear shallow water equations that restores the discrete vector calculus properties. The exploration will be via discrete Fourier dispersion analysis as well as numerical implementation using the Firedrake code generation system (`firedrake-project.org`).

This project will enable the student to get experience of pen-and-paper analysis of finite element discretisations, including the compatible finite element and pressure robust frameworks.

Waves in Photonic and Phononic Crystals

Prof. Richard Craster and Dr. Mehul Makwana

Project Definition

This project is about extraordinary wave transport properties within continuum electronic and acoustic systems, which have various applications to opto-electronic devices. Quite remarkably it is becoming possible to design materials with properties that are not possible in nature, examples being materials with negative e
ective mass, or negative refractive index; these are being used in de-vices. Our aim is to model these exotic materials, design new ones, and interact with groups that build devices. This can be approached from several di
erent angles, each could be a project in its own right:

- Engineering mathematics: There are numerous modelling problems involving waves propagating through finite "crystals" of microstructured materials and these can be approached analytically, using asymptotic methods or numerically.
- Scientific computation: We are developing software to solve these problems systematically in a general manner. The numerical algorithms are based on applied mathematical methods and there is scope to generalise the methods and implement them.
- Mathematical modelling: Concepts often seen in a mathematics degree, such as group theory, are very useful when dealing with periodic media on a lattice. This does not require a deep Pure mathematics knowledge of group theory, but is an application of it to an area of physics. By manipulating the symmetries of the lattice structure unidirectional edge states can be produced and their effects amplified. So there is scope for a mathematics project that draws upon these ideas and blends it with the physics application.
- Mathematical physics: The area of topological insulators in solid state physics and condensed matter theory is vibrant and many exciting ideas are emerging, one of which "topologically protected edge states" has been very influential. The ideas behind this are now moving into other areas of physics such as the photonic and phononic crystals. There are differences when dealing with the continuum cases and there is scope here for moving

ideas from quantum mechanics to continua and we want to explore this aspect.

There will be opportunities to interact with a vibrant research group and attend weekly group meetings. The project could also involve collaboration with the Physics department or a company that designs these materials.

Spectral methods to determine leaky waves in engineering
Professor Richard Craster

This is a project motivated by a need to determine how waves propagate in pipes or waveguides; these are used in the non-destructive evaluation of real structures and in crack detection. A key part of understanding the signal is determining dispersion curves that relate frequency to wavenumber. In essence these are found from an eigenvalue problem and a numerical method called spectral collocation has become popular [1]. This has been extended in many directions, i.e. [2], and forms part of commercial codes nowadays. It is a nice example of mathematics, i.e. spectral methods, orthogonal polynomials, pdes and odes, and scientific computing finding their way into a real application.

The current algorithms do not efficiently tackle so-called leaky waves, i.e. when a waveguide is embedded in another medium then some energy "leaks" into it. This project aims to make algorithms capable of this and will involve a range of applied mathematics tools and some numerical work in either python or matlab.

This project could involve interaction with a world-leading group in Mechanical Engineering who work on non-destructive evaluation.
Algorithms from the mathematics department are in use for dispersion relation calculation both in academia and industry.

[1] A. T. I. Adamou and R. V. Craster, ``Spectral methods for modelling guided waves in elastic media '', J. Acoust. Soc. Am. 116, 1524--1535, 2004 http://dx.doi.org/10.1121/1.1777871

[2] F. Hernando Quintanilla, M. J. S. Lowe and R. V. Craster``Full 3D Dispersion Curve Solutions for Guided Waves in Generally Anisotropic Media'' J. Sound Vib., 363}, 545--559, 2015 https://spiral.imperial.ac.uk:8443/handle/10044/1/2810

Relativistic Path Integrals (Dr Christopher Ford)

Background

Quantum mechanics is normally formulated through a Schrödinger equation involving a Hamiltonian operator. This operator is a quantum counterpart of the classical Hamiltonian. Building on Dirac's work Feynman developed an alternative formulation of quantum mechanics based on the Lagrangian [1]. Here one considers the phase

$$\exp(iS/\hbar) = \exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2} L\ dt\right),$$

for a trajectory with initial time t_1 and final time t_2. One then sums over *all* possible trajectories with specific initial and final boundary conditions. This 'sum' or path integral yields a 'kernel' which is also a solution of Schrödinger's equation.

In many cases the path integral approach is more clumsy than directly applying the Schrödinger equation. However, path integrals are particularly well adapted to relativistic problems. This is because a Hamiltonian treatment singles out time whereas space and time can be treated on an equal footing through a Lagrangian. Path integrals have also proved useful in the study of relativistic quantum field theories. An interesting approach is taken in the textbook of Bailin and Love [2] who start with the Gaussian integral

$$\int_{-\infty}^{\infty} dy\ \exp(-\tfrac{1}{2}ay^2) = (2\pi)^{1/2}a^{-1/2},$$

and develop in turn the theory of path integrals and quantum field theory.

Objectives

To understand the path integral formulation of non-relativistic quantum mechanics. To study in detail the application of the path integral to a relativistic problem. For example, the theory of (a) propagators in curved space or (b) the photon propagator in Quantum Electrodynamics.

References

[1] R. P. Feynman and A. R. Hibbs, 'Quantum Mechanics and Path Integrals'. Emended Edition by D. F. Styler, Dover (2010).

[2] D. Bailin and A. Love, 'Introduction to Gauge Fied Theory Revised Edition', CRC Press (1993).

Quantum dynamical transitions through exceptional points

(Dr E. M. Graefe and Dr S. Malzard)

Systems with time-dependent parameters play an important role in many applications of quantum mechanics. In particular the probability of ending up in a given eigenstate at a final time, when starting in another (or the same) eigenstate at an initial time, is an information that is often useful. It is, however, often challenging to make analytic statements about the solutions of the Schrödinger equation with time-dependent Hamiltonians. Thus, analytically solvable model systems play an important role in approximating and understanding more complicated realistic systems. A prime example is the probability to cross between two instantaneous eigenstates close to a narrow avoided crossing, which can be well described by what is known as the Landau-Zener formula, arising from a simplified model.

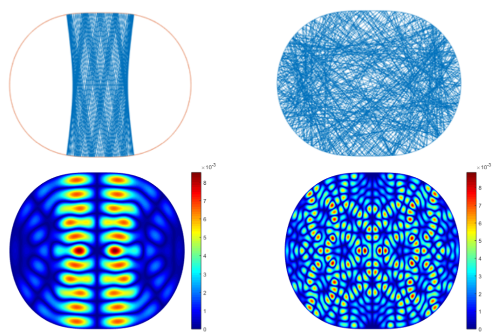
In recent years, there has been much interest in quantum systems with gain and loss, described by non-Hermitian Hamiltonians. The features of such systems are very different from standard Hermitian systems, and many of them remain unstudied hitherto. The difference of Hermitian and non-Hermitian systems is most pronounced in the presence of so-called exceptional points, points in parameter space, at which two or more of the eigenvectors coalesce, a phenomenon that cannot happen for Hermitian operators. In this project we will investigate various generalisations of the Landau-Zener model, for non-Hermitian Hamiltonians, when the system is driven through exceptional points. The quantum physics of non-Hermitian Hamiltonians currently receives a lot of attention, and the provision of new Landau-Zener type equations is expected to be of great relevance for the field. Thus, this project offers a real scope for meaningful scientific discoveries.

While this project does not require a big amount of background knowledge, a minimum working knowledge of quantum mechanics is an important prerequiste.

Quantum billiards with PT-symmetric absorption

(Dr E. M. Graefe and Dr J. Eastman)

The striking difference between quantum and classical behaviour becomes most apparent in the realm of chaos, an extreme sensitivity to initial conditions, which is common in classical systems but impossible under quantum laws. The investigation of characteristic features of quantum systems whose classical counterparts are chaotic lies at the heart of the flourishing research area of quantum chaos. One common example system for the comparison of quantum counterparts of classically chaotic systems are so-called quantum billiards, corresponding to a particle moving freely in a two-dimensional area bounded by different shapes (See the figure on the right for an example of an oval billiard with some classical trajectories and quantum eigenfunctions.). Depending on whether the corresponding classical problem is chaotic or regular, one finds different characteristic behaviours in the eigenfunctions and the eigenvalues of the quantum system. Both can also be accessed experimentally using microwave cavities. On the other hand, the surprising properties of quantum systems with balanced gain and loss (non-Hermitian, but PT-symmetric systems) have sparked much interest recently, and new experimental areas (involving for example optical wave guides, cold atoms, and meta materials) are rapidly emerging. Here we are interested in the hitherto nearly unexplored interplay of chaos and PT-symmetry.



Classical trajectories (top) and quantum probability densities of selected eigenfunctions (bottom) for an oval billiard.

In this project you will investigate the quantum and classical features of PT-symmetric generalisations of quantum billiards. Much of this will be based on numerical simulations, accompanied by analytical calculations and interpretations. This area is of great interest for the scientific community, but so far nearly unexplored. Thus, the project offers a great scope for making new and interesting discoveries.

While this project does not require a big amount of background knowledge, a minimum working knowledge of quantum mechanics and a willingness to use numerical tools are important prerequistes.

Projects in automated numerical PDE methods – Dr David Ham

The numerical solution of PDEs is a key problem of mathematical computing. Many of the largest supercomputers are dedicated to this task for applications including weather forecasting, engineering design, and financial instrument pricing. As simulation scale and sophistication has in- creased, the combination of numerical analysis, parallel algorithms and complex software engineering required has frustrated advances in this field. However, in recent years a radical new approach has emerged. The PDE to be solved, along with its discretisation, are specified in a high level symbolic mathematics language. High performance parallel implementations are then created using specialised compilers, which combine domain knowledge with cutting edge advances in parallel code generation. Students choosing these projects have the opportunity to work on complex mathematical problems while gaining the experience of contributing to professionally engineered open source mathematical software as an integral part of the Firedrake development team (http://firedrakeproject.org). The results of their work will be incorporated into released software in production use at institutions around the world. All of the projects detailed below have the potential, if executed well, to produce results publishable as journal papers. Each project combines a core of numerical mathematics with significant programming, so some level of knowledge of a language such as Python or C is a requirement.

Dual evaluation of finite element spaces.

One core feature that is presently missing in the symbolic levels of Firedrake is the ability to perform dual evaluation: akin to integration of functions. This project will develop the necessary symbolic algebra and representations to enable reasoning about the numerical dual evaluation schemes that Firedrake already uses. The goal is to exploit structure to provide optimal complexity implementations. In particular, we will do this in the Python package FInAT (https://github.com/finat/finat).

Automated differentiation for inverse problems

Inverse problems are pervasive in science and engineering: the forward simulation answers the question “what happens if?” while the inverse problem ask “what was the cause?”. In fields as diverse as climate science and financial mathematics, we need to invert simulations to find the causes of phenomena. In engineering, optimal design requires inverse simulations to design the system which best produces a desired outcome.

A key requirement in inverse simulation is to differentiate the model. For an automated system such as Firedrake, this requires the symbolic mathematics code that Firedrake programs are written in to be differentiated automatically using techniques from computer algebra. Many parts of Firedrake are already automatically differentiable, but important holes remain. This project will enable a student to learn about inverse simulation techniques while contributing new automatic differentiation capabilities to the Firedrake system.

Spatio-temporal vaccine coverage estimation in Nigeria
Dr Alex de Figueiredo & Dr Nick Jones

Incomplete coverage of routine childhood immunisations (such as the childhood measles-mumps-rubella, polio, or diphtheria-tetanus-pertussis vaccines) cause preventable illness, death, and economic burdens. In a number of settings worldwide, losses in trust in vaccination programmes has decreased immunisation rates, increasing disease burdens. Over the past few years, collection of large-scale household level survey data with spatial information has permitted the estimation of vaccine coverage at fine spatial scales [1,2]. These models, however, do not account for parents that may have incorrectly reported their children as being vaccinated. Not accounting for parental recall error may result in inflation of vaccine coverage estimates: indeed, recent evidence suggests that there may be up to a 10% difference in vaccine coverage from that inferred in models and the 'ground-truth' coverage levels [3].

In this project, you will use tools from machine learning to estimate and forecast immunisation rates at the sub-national level in Nigeria accounting for this parental recall bias. Using survey data from the Demographic and Health Surveys data [4], you will provide spatio-temporal vaccine coverage estimates across Nigeria over multiple time points. This project will expose you to statistical forecasting models (Gaussian processes [5]), methods for model validation (the training-testing paradigm), and computational methods (Gibbs sampling [6]) for model inference. The research is expected to lead to publishable insights on the effect of recall bias on immunisation estimates.

Programming skills: Python or R required.

[1] Utazi et. al. High resolution age-structured mapping of childhood vaccination coverage in low and middle income settings *Vaccine* (2018)
[2] Mosser et. al. Mapping diphtheria-pertussis-tetanus vaccine coverage in Africa, 2000-2016: a spatial and temporal modelling study *The Lancet* (2019)
[3]. Gong et. al. Using serosurvey data triangulation for more accurate estimates of vaccine coverage: measured and modelled coverage from Pakistan household surveys. *Am. J. Epidem.* (2019)
[4] www.dhsprogram.com
[5] Rasmussen and Williams. Gaussian Processes for Machine Learning. MIT Press. 2016
[6] Brooks, et. al. Handbook of Markov Chain Monte Carlo. Chapman & Hall/CRC. 2011.

Dr Eric Keaveny

Sedimentation of flexible filaments

Sedimentation — the motion of particles in viscous fluids due to gravity — is one of the most commonplace situations imaginable. Despite this, it is at the same time rather complicated due to long-ranged hydrodynamic interactions between particles. This situation become more complex when the particles are also deformable and can change shape in response to hydrodynamic stresses. This project uses computational models to explore this situation in the context of flexible filaments that can bend and twist. The project entails examining how filament flexibility affects the sedimentation of isolated filaments, as well as small groups.

Stability of active filaments

In biology, actuated filaments, such as flagella or cilia, are commonly used to pump fluid, or propel cells. While the internal structure of these filaments is well documented, what is still not entirely clear is how emergent filament motion is linked to its underlying internal actuation. The project entails using computational models to ascertain whether resulting 3D waveforms can result from the instability of 2D actuation, or whether a fully 3D actuation strategy is required. While this project will focus primarily on single filament simulations, there is also scope to explore how the actuation affects synchrony with other nearby filaments.

Multiscale hydrodynamic interactions

Microorganisms and swimming cells often use time-dependent deformations of their bodies to generate the flows needed to propel themselves from one place to another. This flow then influences the motion of nearby organisms that are also deforming themselves. This project entails exploring the non-trivial coupling between the time-dependent flows and shape changes and how it affects hydrodynamic interactions. The project will begin by exploring the interactions between two simple model swimmers.

Dr Adam Townsend

Particle suspensions moving through confined spaces (with Dr Eric Keaveny)

Fluids move differently to solids, in part because of their ability to be funnelled. So while a liquid can move through a funnel quite happily, any solid particles suspended in the fluid may be rearranged in order to pass through.

Fluids with solid particles suspended in them are common in nature and industry: ceramics, paint, blood, and concrete, to name a few, can all be characterised as viscous fluids in which small particles are distributed. As part of their application, these particle suspensions often find themselves being transported through pipes or channels, which sometimes have varying widths.

This project looks at concentrated particle suspensions as they pass through funnels. If the funnel angle is very shallow, the particles will pass through almost undisturbed. Too steep, and the particles will simply clog the outlet. Experimental data shows, for certain funnel angles and concentrations, shockwaves passing backwards through the oncoming suspension. We will use computer models to try to reproduce this behaviour and perhaps go on to try more interesting funnel shapes.

This is a computational project using code written in Python and some comfort with programming is required.

MSc in Applied Mathematics Research Project: Topological data analysis of election outcomes

Supervision: Florian Klimm & Nick Jones

Recommended Prerequisites

- 'Methods for Data Science'
- 'Introduction to Machine Learning'
- Programming in PYTHON
- Knowledge/interest in UK politics
- Topology and Statistics (solid foundations are beneficial)

Aim

In this project, we investigate to what extent tools that have been developed for the analysis of single-cell RNA-sequencing data can lead to insights on election data. Among these tools are dimensionality-reduction methods (e.g., tSNE, PCA), clustering techniques (e.g., modularity maximisation), and trajectory-inference approaches.

Focus of this project is *not* the development of novel statistical methods but rather the application of existing tools that are available in the python library SCANPY [1].

Background

We can represent election results for p parties in c constituencies in a vote share matrix

$$\mathbf{V} = [0, 1]^{p \times c}\,, \tag{1}$$

where each element V_{ij} indicates the share of votes that party i obtained in constituency j. Similar matrices occur in the analysis of single-cell RNA-sequencing measurements in which the element V_{ij} indicates the expression of gene i in cell j. Therefore, the applications of machine-learning techniques that have been developed for single-cell RNA sequencing data to voting data could be fruitful.

Dimensionality-reduction methods, such as *Uniform Manifold Approximation and Projection* (UMAP [2]), can be used to visualise and investigate such high-dimensional data (see Fig. 1). UMAP is based on the estimation of fuzzy topological structures from the data.

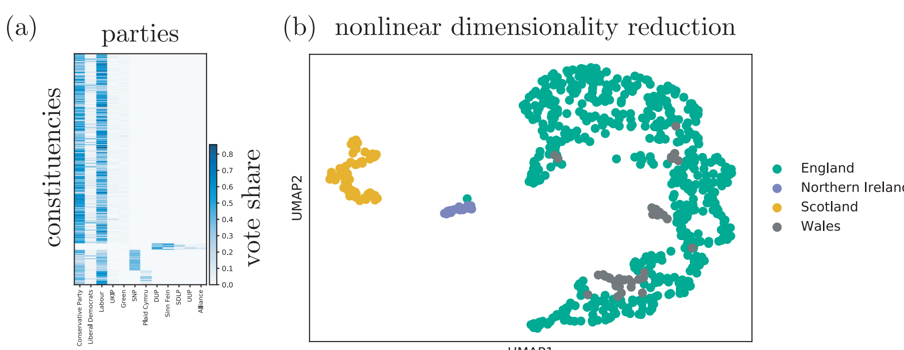


Figure 1: (a) We represent the election results of the 2017 general election as a vote share matrix $\mathbf{V}$ in which columns represent parties and rows represent constituencies. (b) In this UMAP plot each disk represents a constituency and their colours indicate the country they belong to.

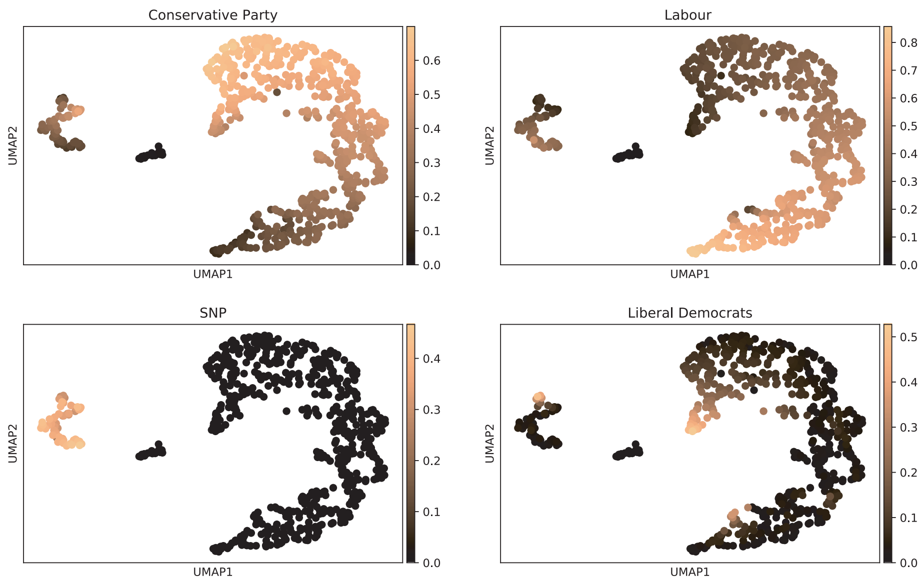


Figure 2: We show the the dimensionality reduction as in Fig. 1. In each panel, the disks' colours indicate vote share for one of the four major parties (Conservative Party, Labour, Scottish National Party, and Liberal Democrats).

Project overview

Analysis of the 2019 General Election

In a first step, we investigate the most recent election results. A crucial part of the investigation is to determine how potential correction steps (e.g., normalisation of parties vote share or batch-correction to compare constituencies of different countries) change the interpretation of results.

A cluster analysis enables us to identify constituencies that have similar election outcomes. The comparison with other data about the constituencies (e.g., population density, Brexit referendum outcome, unemployment rate) allows us to quantify the relevance of these cofactors in a statistically meaningful way.

Temporal analysis

The *House of Commons Library* makes the election results from 1918 to 2019 available. Using tools such as *trajectory analysis* we describe temporal trends. A particular focus is the comparison with other metadata to test whether common narratives (e.g., an increasing divergence between rural and urban areas) are statistically significant on a 100 year time scale.

Optional further research directions

Extension to other countries

These results could be extended with the analysis of other countries, depending on the student's expertise. For Germany one could, for example, test to what extent an East–West electoral division is still statistically significant and whether it is changing over time. For the US, we could investigate whether common classifications of electoral districts (rural, suburban, and urban) are statistically justified.

References

[1] F Alexander Wolf, Philipp Angerer, and Fabian J Theis. SCANPY: Large-scale single-cell gene expression data analysis. *Genome Biology*, 19(1):15, 2018.

[2] Leland McInnes, John Healy, and James Melville. Umap: Uniform manifold approximation and projection for dimension reduction. *arXiv preprint arXiv:1802.03426*, 2018.

MSc project proposals: Prof Jeroen S.W. Lamb

Set-valued analysis of bifurcations in random systems with bounded noise.

Random dynamical systems with bounded noise typically have stationary measures that are supported on bounded so-called minimal invariant sets. Stationary measures describe the statistics of random systems. The aim is to develop efficient numerical methods to approximate these minimal invariant sets, and track these sets while they change continuously when parameters are varied. A second challenge concerns bifurcations where minimal invariant sets change discontinuously at certain parameter values. We aim to predict such bifurcations before they are about to happen. The project should focus on one of these two aspects, extending and improving rudimentary algorithms that are currently working for prototypical examples only. Down the line, these kind of methods will be important for uncertainty quantification and the understanding of mechanisms underlying rapid drastic changes (tipping points). There are theoretical and numerical challenges to be addressed. (This project will be potentially co-supervised by Dr Rasmussen and PhD students Wei-Hao Tey and Kalle Timperi.)

Conditioned random dynamics.

The aim of this project is to describe spatially localised properties of random system through conditioning to a bounded region and the existence of quasi-ergodic and/or quasi-stationary measures for the latter process. In this context, one may define dynamical properties such as conditional Lyapunov exponents that characterise the system on a local rather than a global spacial scale. The project will address the connection between dynamical and statistical features and may range from theoretical analysis of elementary examples to numerical explorations. (This project will be potentially co-supervised by Dr Rasmussen and PhD student Guillermo Olicon Mendez.)

Attractor reconstruction from high-dimensional infrequent data.

In this project we study a novel method to learn dynamics from high-dimensional infrequent data samples, based on so-called Takens embedding. This method has shown great promise and potential practical relevance, eg for health care or other applications where it is impractical to obtain long time-series, but where infrequent measurements can contain a lot of observables. The project will deal with several practical challenges inherent to this method.

References:

H Ma, T Zhou, K Aihara, L Chen. Predicting time series from short-term high-dimensional data, International Journal of Bifurcation and Chaos **24**, 1430033 (2014)

H Ma, K Aihara, L Chen. Detecting causality from nonlinear dynamics with short-term time series. Scientific reports **4**, 7464 (2014)

MSc Projects

1. Curve evolutions on tori via conformal maps

Given a curve in a two-dimensional Riemannian manifold $(\mathcal{M}, g)$ that is conformally flat, we can define curvature flow and elastic flow as

$$\mathcal{V}_g = -\varkappa_g \tag{1}$$

and

$$\mathcal{V}_g = -(\varkappa_g)_{s_g s_g} - \tfrac{1}{2}\,\varkappa_g^3 - S_0\,\varkappa_g\,, \tag{2}$$

respectively. Here $\varkappa_g$ is the geodesic curvature, $\mathcal{V}_g$ is the normal velocity of the curve with respect to the metric g, $\partial_{s_g} = g^{-\frac{1}{2}}\,\partial_s$, s denoting arclength, and S_0 is the sectional curvature of g.

A special application is when the metric is induced by a conformal parameterization $\vec\Phi : H \to \mathbb{R}^d$, $d \geq 3$, of the two-dimensional Riemannian manifold $\mathcal{M} \subset \mathbb{R}^d$, i.e. $\mathcal{M} = \vec\Phi(H)$ and $|\partial_{\vec e_1}\vec\Phi(\vec z)|^2 = |\partial_{\vec e_2}\vec\Phi(\vec z)|^2$ and $\partial_{\vec e_1}\vec\Phi(\vec z)\,.\,\partial_{\vec e_2}\vec\Phi(\vec z) = 0$ for all $\vec z \in H$. Here examples include the stereographic projection of the unit sphere, without the north pole, onto the plane,

$$\vec\Phi(\vec z) = (1 + |\vec z|^2)^{-1}\,(2\,\vec z\,.\,\vec e_1, 2\,\vec z\,.\,\vec e_2, |\vec z|^2 - 1)^T\,,$$
$$g(\vec z) = 4\,(1 + |\vec z|^2)^{-2} \quad \text{and} \quad H = \mathbb{R}^2\,; \tag{3a}$$

the Mercator projection of the unit sphere without the north and the south pole,

$$\vec\Phi(\vec z) = \cosh^{-1}(\vec z\,.\,\vec e_1)\,(\cos(\vec z\,.\,\vec e_2), \sin(\vec z\,.\,\vec e_2), \sinh(\vec z\,.\,\vec e_1))^T\,,$$
$$g(\vec z) = \cosh^{-2}(\vec z\,.\,\vec e_1) \quad \text{and} \quad H = \mathbb{R}^2\,; \tag{3b}$$

as well as the catenoid parameterization

$$\vec\Phi(\vec z) = (\cosh(\vec z\,.\,\vec e_1)\,\cos(\vec z\,.\,\vec e_2), \cosh(\vec z\,.\,\vec e_1)\,\sin(\vec z\,.\,\vec e_2), \vec z\,.\,\vec e_1)^T\,,$$
$$g(\vec z) = \cosh^2(\vec z\,.\,\vec e_1) \quad \text{and} \quad H = \mathbb{R}^2\,. \tag{3c}$$

We also recall the following conformal parameterization of a torus with large radius $R > 1$ and small radius $r = 1$. In particular, we let $\mathfrak{s} = [R^2 - 1]^{\frac{1}{2}}$ and define

$$\vec\Phi(\vec z) = \mathfrak{s}\,([\mathfrak{s}^2 + 1]^{\frac{1}{2}} - \cos(\vec z\,.\,\vec e_2))^{-1}\,(\mathfrak{s}\,\cos\tfrac{\vec z\,.\,\vec e_1}{\mathfrak{s}}, \mathfrak{s}\,\sin\tfrac{\vec z\,.\,\vec e_1}{\mathfrak{s}}, \sin(\vec z\,.\,\vec e_2))^T\,,$$
$$g(\vec z) = \mathfrak{s}^2\,([\mathfrak{s}^2 + 1]^{\frac{1}{2}} - \cos(\vec z\,.\,\vec e_2))^{-2} \quad \text{and} \quad H = \mathbb{R}^2\,. \tag{3d}$$

See [BGN] for details. We note that in the examples (3c) and (3d), any closed curve $\vec x(I)$ in H will correspond to a curve $\vec\Phi(\vec x(I))$ on the hypersurface $\mathcal{M}$ that is homotopic to a point. In order to model other curves, the domain H needs to be embedded in an algebraic structure different to $\mathbb{R}^2$. In particular, $H = \mathbb{R} \times \mathbb{R}/(2\,\pi\,\mathbb{Z})$ for (3c) and $H = \mathbb{R}/(2\,\pi\,\mathfrak{s}\,\mathbb{Z}) \times \mathbb{R}/(2\,\pi\,\mathbb{Z})$ for (3d), respectively. For the implementation that means that all the calculations, e.g. vector addition, scalar multiplication, the distance function, need to be performed in e.g. $H = \mathbb{R}/(2\,\pi\,\mathbb{Z}) \times \mathbb{R}/(2\,\pi\,\mathbb{Z})$ for the Clifford torus, rather than in $\mathbb{R}^2$.

Prerequisites: Some knowledge of finite elements or finite differences. Programming skills, including operator overloading in C++ or Python.

References

[BGN] John W. Barrett, Harald Garcke, and Robert Nürnberg. Numerical approximation of curve evolutions in Riemannian manifolds, 2018. http://arxiv.org/abs/1809.01973.

2. Image segmention and image restoration with active contours

Two fundamental tasks in image processing are image segmentation and image smoothing. A natural strategy is to combine the two processes in a single step, following the idea of the seminal work by [MS]. They introduced the following optimization problem: Find a minimizer (u, S) of the functional

$$E_{\rm MS}(u, S) = \sigma\, \mathcal{H}^{d-1}(S) + \lambda \int_\Omega (u - u_0)^2 \,{\rm d}\mathcal{L}^d + \int_{\Omega\setminus S} |\nabla\, u|^2 \,{\rm d}\mathcal{L}^d \,. \qquad (1)$$

Here, given an image $u_0 : \mathbb{R}^d \supset \Omega \to \mathbb{R}$, the task is to find its set of discontinuities S, and a piecewise smooth approximation $u : \Omega \to \mathbb{R}$ of u_0.

As the Mumford–Shah problem is difficult to tackle in its original form, several simplified models have been proposed. Chief among them are the models by [CV] and [TYW] which, in their simplest forms, assume that S is a closed curve Γ that partitions Ω into two regions: Ω_1 and Ω_2. Moreover, u is assumed to be constant or smooth in each of the two regions. Hence (1) reduces to

$$E(u, \Gamma) = \sigma\, \mathcal{H}^{d-1}(\Gamma) + \lambda \sum_{i=1}^{2} \int_\Omega (u_i - u_0)^2 \,{\rm d}\mathcal{L}^d + \sum_{i=1}^{2} \int_{\Omega_i} |\nabla\, u_i|^2 \,{\rm d}\mathcal{L}^d \,. \qquad (2)$$

Possible numerical approaches to minimize (2) can be found in e.g. [DMN] and [Ben], where the latter work uses a piecewise constant approximation of u and active contours based on [BGN]. The aim of this project is to build on the work in [Ben], but with $u = u_1\, \mathcal{X}_{\Omega_1} + u_2\, \mathcal{X}_{\Omega_2}$ being a piecewise smooth approximation.

Prerequisites: Good knowledge of finite differences and finite elements. Programming skills in C, MATLAB or Python.

References

[Ben] Heike Benninghoff. *Parametric Methods for Image Processing Using Actice Contours with Topology Changes.* PhD thesis, University Regensburg, Regensburg, 2015.

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[CV] T. F. Chan and L. A. Vese. Active contours without edges. *IEEE Trans. Image Process.*, 10(2):266–277, 2001.

[DMN] Günay Doğan, Pedro Morin, and Ricardo H. Nochetto. A variational shape optimization approach for image segmentation with a Mumford-Shah functional. *SIAM J. Sci. Comput.*, 30(6):3028–3049, 2008.

[MS] David Mumford and Jayant Shah. Optimal approximations by piecewise smooth functions and associated variational problems. *Comm. Pure Appl. Math.*, 42(5):577–685, 1989.

[TYW] A. Tsai, Jr. Yezzi, A., and A. S. Willsky. Curve evolution implementation of the Mumford–Shah functional for image segmentation, denoising, interpolation, and magnification. *IEEE Trans. Image Process.*, 10(8):1169–1186, 2001.

Numerical solution of fractional diffusion

Supervisor: Dr Sheehan Olver

The classic diffusion/heat equation is of course given by

$$u_t = u_{xx} \qquad \text{and} \qquad u(0,x) = u_0(x).$$

The *fractional diffusion equation* replaces the time-derivative by a fractional variant

$$D_t^r u = u_{xx} \qquad \text{and} \qquad u(0,x) = u_0(x).$$

where r is say a rational number and D_t^r denotes the (Caputo) fractional derivative. The precise definition is in terms of the fractional integral

$$Q_t^r f(t) = \frac{1}{\Gamma(r)} \int_0^t \frac{f(\tau)}{(t-\tau)^{1-r}} \, \mathrm{d}\tau$$

and then

$$D_t^{m+r} f(t) := Q_t^{1-r} \frac{\mathrm{d}^{m+1}}{\mathrm{d}t^{m+1}} f(t)$$

where m is an integer (that is, we differentiate and then do a fractional integral). It may not be completely obvious, but this does in fact reduce to standard derivatives for integer r.

Fractional diffusion equations arise in a number of applications including mathematical finance and medical imaging. The rough reason why is that the fractional derivative operator is *nonlocal*: it depends on the solution for all previous times (going back to $t = 0$), hence are useful in applications with *memory*: e.g., financial modelling where history is used or medical imagining where tissue changes over time.

This project is to investigate solving such equations, first with periodic boundary conditions in x using Fourier series. This reduces the problem to fractional ordinary differential equations, which may be tackled using recent results of mine with Nick Hale on spectral methods for fractional differential equations, built out of special orthogonal polynomial relationships. This is perhaps not as straightforward as it sounds: there are issues with bad conditioning that must be worked around. Further extensions to other spatial boundary conditions (Dirichlet or Neumann) and nonlinear fractional diffusion equations, including challenging cases arising in applications, will then be considered.

Partial differential equations on three-dimensional simplices via multivariate orthogonal polynomials

Supervisor: Dr Sheehan Olver

In recent work, myself, Townsend, and Vasil have introduced an approach to solving partial differential equations on triangles using a hierarchy of multivariate orthogonal polynomials. For example, on the right triangle $T = \{(x,y) : 0 \le x, y \le 1, 0 \le x+y \le 1\}$, we consider orthogonal polynomials with respect to the inner product

$$\iint_T f(x,y) g(x,y) x^a y^b (1-x-y)^c \, \mathrm{d}A.$$

General linear partial differential equations such as the the variable coefficient Helmholtz equation

$$\Delta u + a(x,y)u = f(x,y), \qquad u|_{\partial T} = 0$$

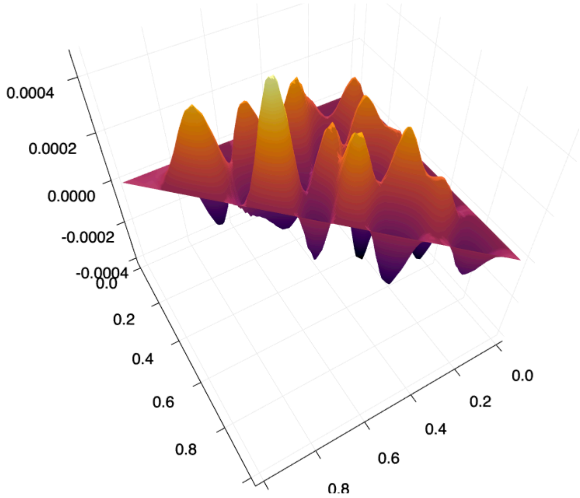

Figure 1: Solution to Helmholtz equation in a triangle.

become *banded-block-banded* equations when we use two different choices of a, b, c for the bases used to represent u and f. An example of a banded-block-banded system would have the zero structure of the form:

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\end{array}\right)
\begin{pmatrix} u_{00} \\ \hline u_{10} \\ u_{11} \\ \hline u_{20} \\ u_{21} \\ u_{22} \\ \hline u_{30} \\ u_{31} \\ u_{32} \\ u_{33} \end{pmatrix}
=
\begin{pmatrix} f_{00} \\ \hline f_{10} \\ f_{11} \\ \hline f_{20} \\ f_{21} \\ f_{22} \\ \hline f_{30} \\ f_{31} \\ f_{32} \\ f_{33} \end{pmatrix}$$

that is, a block tridiagonal matrix whose the blocks themselves are also tridiagonal. The sparsity present in this structure allows for extremely high polynomial order approximation methods, with as many as 100k unknowns. An example solution is given in Figure 1 for the Helmholtz equation.

The MSc. project consists of extending this methodology to solve PDEs on three-dimensional simplices, e.g., $S = \{(x, y, z) : 0 \leq x, y, z \leq 1, 0 \leq x + y + z \leq 1\}$, using multivariate orthogonal polynomials with respect to the inner product

$$\iiint_S f(x, y, z) g(x, y, z) x^a y^b z^c (1 - x - y - z)^d \, \mathrm{d}V$$

where choosing (a, b, c, d) differently will reveal an underlying sparsity structure. The project will involve generalising the recurrence relationships derived for two-dimensional multivariate orthogonal polynomials to three-dimensions, using these to construct matrix representations of the operators, and solving some simple model problems like three-dimensional Poisson equation and Helmholtz equations.

Project 1: **(Prof G.A. Pavliotis and Dr. U.P. Vaes) Optimal control for opinion formation models**. Multiagent systems are often used to model different processes in the social sciences such as pedestrian dynamics, wealth distribution, systemic risk, the evolution of urban areas and opinion formation. Mathematical models for opinion formation are often based on systems of (weakly) interacting agents in the presence of noise, modelling uncertainty. Such models, in the (mean field) limit of infinitely many agents, exhibit a transition from a uniform distribution of opinions to consensus, depending on the strength of the interaction between the agents, that can be thought of as a disorder-order phase transition. A natural question is then whether consensus can be achieved by means of optimal control of the dynamics. The goal of this project is to develop and implement optimal control methodologies for stochastic models for opinion formation, using tools from numerical analysis for PDEs and from optimal control theory for diffusion processes.

Bibliography

Heterophilious dynamics enhances consensus S Motsch, E Tadmor SIAM review 56 (4), 577-621

Mean-field limits for interacting diffusions with colored noise: phase transitions and spectral numerical methods SN Gomes, GA Pavliotis, U Vaes arXiv preprint arXiv:1904.05973

Noisy Hegselmann-Krause Systems: Phase Transition and the 2*R*-Conjecture C Wang, Q Li, E Weinan, B Chazelle Journal of Statistical Physics 166 (5), 1209-1225

Project 2: (Prof G.A. Pavliotis) **The Ito versus Stratonovich dilemma, inference and population dynamics.** Stochastic differential equations (SDEs) are routinely used as mathematical models in the natural and social sciences, such as physics, chemistry, biology and finance. A very interesting application of stochastic differential equations is to mathematical models in population dynamics. A standard example of SDEs used in population dynamics is that of coupled Lotka-Volterra systems driven by multiplicative noise. A crucial question is how to model the noise. It is well known that different interpretations of the stochastic integral, e.g. Ito or Stratonoich can lead to SDEs with different qualitative properties. The purpose of this project it twofold: first, to develop inference methodologies for identifying the correct interpretation of noise using data. Second, the systematic study of the effect of different interpretations of the stochastic integral on the stability properties of coupled Lotka-Volterra systems.

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Mao, Xuerong, Sotirios Sabanis, and Eric Renshaw. "Asymptotic behaviour of the stochastic Lotka–Volterra model." *Journal of Mathematical Analysis and Applications* 287.1 (2003): 141-156.

Pavliotis, G. A., and A. M. Stuart. "Parameter estimation for multiscale diffusions." *Journal of Statistical Physics* 127.4 (2007): 741-781.

Braumann, Carlos A. "Growth and extinction of populations in randomly varying environments." *Computers & Mathematics with Applications* 56.3 (2008): 631-644.

Bo, Stefano, and Antonio Celani. "White-noise limit of nonwhite nonequilibrium processes." *Physical Review E* 88.6 (2013): 062150.

Morse decompositions of nonautonomous set-valued dynamical systems (Dr Rasmussen)

The global asymptotic behaviour of dynamical systems on compact metric spaces can be described via Morse decompositions. Their components, the so-called Morse sets, are obtained as intersections of attractors and repellers of the system. This project aims at generalisations of the classical theory to dynamical systems that are both nonautonomous and set-valued, by extending results from [1], [2] and [3]. [1] R.P. McGehee and T. Wiandt, Conley decomposition for closed relations, Journal of Difference Equations and Applications 12 (2006), no. 1 1-47. [2] M. Rasmussen, Morse decompositions of nonautonomous dynamical systems, Transactions of the American Mathematical Society 359 (2007), no. 10, 5091-5115.

[3] Yejuan Wang, Desheng Li, Morse Decompositions for Nonautonomous General Dynamical Systems, Set-Valued and Variational Analysis 22 (2014), 117-154.

Approximation of nonautonomous invariant manifolds (Dr Rasmussen)

In nonlinear dynamical systems, invariant manifolds are omnipresent and play a crucial role in a variety of ways for local as well as global questions: For instance, local stable and unstable manifolds dictate the saddle point behaviour in the vicinity of hyperbolic solutions (or surfaces), and center manifolds are a primary tool to simplify given dynamical systems in terms of a reduction of their state space dimension. Concerning a more global perspective, stable manifolds serve as separatrix between different domains of attractions. This project aims at computing invariant manifolds for time-variant discrete dynamical systems numerically, by using and extending results from [1]. Here a truncation of the Lyapunov-Perron operator, used for the construction of invariant manifolds, results in a system of nonlinear algebraic equations which can be solved both locally using Newton, and globally using continuation algorithms, yielding both local and global approximations of the desired invariant manifold. The project aims in particular at using continuation techniques to study approximations of one- and two-dimensional invariant manifolds.

References: [1] C. Poetzsche and M. Rasmussen, Computation of nonautonomous invariant and inertial manifolds, Numerische Mathematik 112 (2009), no. 3, 449-483.

Approximation of quasi-ergodic measures for random dynamical systems (Professor Lamb and Dr Rasmussen)

Recent work by our PhD student Maximilian Engel identified the need to approximate quasi-ergodic measures for random dynamical systems. The overall aim is to describe spatially localised statistical properties of the random system. We propose to use a modified version of Ulam's method - a course graining approximation - for this purpose. Ulam's method is typically used to compute global statistical properties, and the approximation of quasi-ergodic measures involves an application of the standard Ulam's method and the additional analysis of a correction term. The overall aim is to use the quasi-ergodic measure to determine dynamical properties such as conditional Lyapunov exponents that characterise the system on a local rather than a global spacial scale. Such applications will be addressed in this project.

Contact networks and disease transmission in pedestrian flows

Supervisor: Dr. Prasun Ray

Project Description

Analysis and optimization of pedestrian flows is fundamentally important for both urban design and public health and safety. 'Great' cities facilitate physical in-person contact [1], however large levels of such contact also lead to higher rates of disease transmission. A challenging design problem follows immediately – how can we generate efficient, high-density, and *safe* pedestrian flows? This project approaches this problem in three steps. First, by simulating pedestrian flows in canonical configurations such as uni- and bi-directional traffic in a hallway using the descision-based model developed in [2]. It is well known that traffic waves and turbulence can develop under certain conditions in these flows, and the second step is to analyze the contact networks that form as waves and turbulence develop. Relevant questions to be considered are: which other walkers does a pedestrian come into contact with? What are the durations of these interactions? The third step is to couple the contact network results to disease transmission models in order to characterize the degree to which simulated traffic facilitates epidemics and the spreading of infectious diseases. There is also substantial scope to move beyond this outline and tailor the project to student interests.

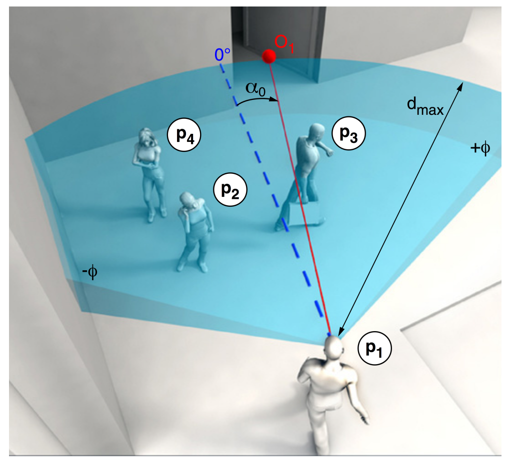


Illustration of a pedstrian (p_1) analyzing her path (taken from [2])

Learning Outcomes

There will be several learning outcomes emerging from this project:
· You will learn about numerical methods for large systems of ODEs and optimzation; you will also acquire proficiency in scientific computing
· You will learn about mathematical epidemiology and network science
· You will also learn about the dynamics of linear and nonlinear waves in the context of pedestrian traffic

Background: The following courses (or equivalent) may be useful, however not all are essential: Hydrodynamic Stability, Numerical Solution of ODEs, Computational PDEs, Scientific Computing. Some programming experience (e.g. Matlab or Python) will be helpful.

References

[1] Sim, A., Yaliraki, S. N., Barahona, M., & Stumpf, M. P. H. (2015). Great cities look small. Journal of The Royal Society Interface, 12(109), 20150315.

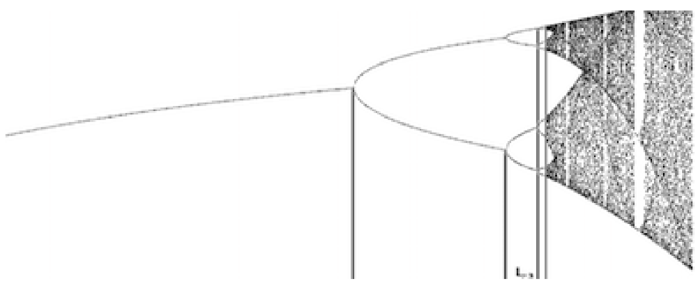
[2] M. Moussaid, D. Helbing, & G. Theraulaz. How simple rules determine pedestrian behavior and crowd disasters. Proc. Natl. Acad. Sci. USA, 108::6884-6888 2011.

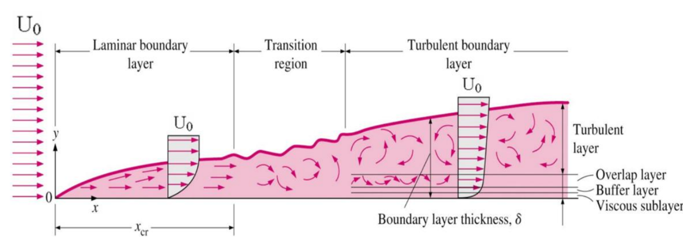
Transition to chaos in model spatially-developing flows

Supervisors: Dr. P. K. Ray and Prof. D. T. Papageorgiou

Project Description

Consider the figure below. The image on the left is a bifurcation diagram for the logistic map, $x_{n+1} = rx_n(1 - x_n)$; this map was analyzed by Feigenbaum 40 years ago in his foundational study on the period-doubling route to chaos [1]. The image on the right illustrates the spatial development of a fluid boundary layer as it *transitions* from a steady, laminar flow to fully-developed turbulence. The basic question motivating this project is, can the bifurcation diagram on the left at all describe the dynamics depicted in the boundary layer on the right? Boundary layers have great practical significance – consider water flowing through pipes in your home, air flow over an aircraft wing, or hurricanes after landfall. While these flows are undoubtedly important, they are also enormously complicated and require simulation and analysis of the 3-D Navier-Stokes equations. In this project, we make a pragmatic compromise and focus on the spatially-developing 2-D Kuramoto-Sivashinsky (K-S) equation, $u_t + (u + c)u_x + \nabla^2 u + \nabla^4 u = 0$, which retains many important features of the Navier-Stokes equations but is simpler to analyze and simulate. Transition to chaos in the K-S system has already been investigated for confined dynamics on a periodic domain, $x \in [0, L)$ [2], and in this project, we will analyze open flows developing along the half line, $x \in [0, \infty)$. Numerical simulations will be used as a 'laboratory' for investigating transition scenarios. Statistical methods and nonlinear time series analysis will be applied to simulation results and connections to insights gained from both chaos theory and linear stability analysis will be explored and explained.





Learning Outcomes

There will be several learning outcomes emerging from this project:
- You will learn about numerical methods for nonlinear PDEs and acquire proficiency in scientific computing
- You will also learn about nonlinear time series analysis and statistical analysis of complex spatio-termporal data
- You will learn about linear stability analysis of spatially developing flows and asymptotic methods used to connect linear theory to observed nonlinear dynamics.

Background: The following courses (or equivalent) from the Applied Mathematics program could prove useful, however not all are essential: Fluid Dynamics I/II, Hydrodynamic Stability, Asymptotic Analysis, Numerical Solution of ODEs, Computational PDEs. Some programming experience is essential.

References

[1] S.H. Strogatz, Nonlinear dynamics and chaos, 2000.

[2] Y.-S. Smyrlis and D.T. Papageorgiou. Predicting chaos for infinite-dimensional systems: The Kuramoto-Sivashinsky equation, a case study. Proc. Natl. Acad. Sci. USA, 88:11129-11132, 1991.

1. Equilibrium and stability of liquid films and drops pinned at sharp edges (Dr Ory Schnitzer)

Consider a liquid film or drop in contact with a smooth solid substrate. In equilibrium, the liquid interface meets the solid substrate at a contact angle which is locally determined by a balance of interfacial tensions (Young-Dupre law). In contrast, if the liquid interface is "pinned" at a sharp edge, local considerations imply an interval of permissible contact angles, the actual value being determined by global considerations. Typically, the interface will detach from the sharp edge as the equilibrium contact angle exits the permissible interval, or if the corresponding equilibrium state becomes unstable. The study of "depinning" transitions is key to understanding the motion of liquid drops and films along rough and textured surfaces, as well as the durability of engineered water-repellent surfaces ("superhydrophobic" surfaces) [1].

In this project you will formulate and analyse, using analytical and numerical methods, mathematical models for calculating equilibrium profiles of pinned liquid films and drops for a range of texture geometries of increasing complexity. You will also use variational principles to study the thermodynamic stability of these equilibrium profiles, with the goal of studying the durability of superhydrophobic surfaces under varying conditions [2]. In addition to exact methods, there is opportunity to employ multiple-scale perturbation methods to bridge the gap between the small scale of the surface texture and typically larger capillary length and drop scale.

[1] D. Quere, Wetting and roughness, Annual Review Material Research, 38, 71 (2008); F. Schellenberger, N. Encinas, D. Vollmer and H. J. Butt, How water advances on superhydrophobic surfaces, Physical Review Letters, 116, 096101 (2016)

[2] J. Bostwick and P. Steen, Stability of constrained capillary surfaces, Annual Review Fluid Mechanics, 47, 539 (2015); J. Grana-Otero and I. E. Parra Fabian, Contact line depinning from sharp edges, Physical Review Fluids, 4, 114001 (2019); J. Grana-Otero and I. E. Parra Fabia, Equilibrium and stability of two-dimensional pinned drops, arXiv:1908.07971.

2. Optical resonances of subwavelength nanoparticles (Dr Ory Schnitzer)

There is practical interest in devising techniques to manipulate light on small scales, in particular smaller than the electromagnetic wavelength, thus "breaking the diffraction limit" of traditional optical apparatus and enabling revolutions in sensing and imaging. One approach is to exploit the unique optical resonances of metallic and high-index dielectric nanoparticles, which occur at wavelengths large compared to particle size (usually particles resonate at wavelengths at most comparable to their size, analogous to the standing waves of a string fixed at both ends) [1]. A general approach to calculating the interaction between electromagnetic waves and resonant particles is to adopt a modal decomposition of the scattered field in terms of "geometric" eigenmodes [2]. The latter are defined through an eigenvalue problem at fixed frequency, the eigenvalue being the value of the particle permittivity such that an outward radiating eigen-solution of Maxwell's equation exists in the absence of any external forcing.

The main challenge with this approach is to compute the eigenvalues and eigenmodes for a given particle geometry over a significant range of frequencies. The goal of this project is to tackle this challenge using asymptotic analysis in the pertinent limit where the particle is small compared to the wavelength. In particular, the method of matched asymptotic expansions [3] can be used to obtain analytical approximations to the eigenvalues and eigenfunctions in terms of a set of geometric parameters determined by simplified shape-dependent canonical problems that in general need to be solved numerically.

[1] S. A. Maier, Plasmonics: fundamentals and applications, Springer (2007); A. I. Kuznetsov et al., "Optically resonant dielectric nanostructures," Science 354 6314 (2016).

[2] D. Bergman and D. Stroud, Theory of resonances in the electromagnetic scattering by macroscopic bodies, Phys. Rev. B, 22 (8) 3527 (1980).

[3] For an application to low-frequency scattering, see Chapter 6 in D. G. Crighton et al., "Modern methods in analytical acoustics," Springer (1992).

Stochastic genetic networks and developmental robustness – Dr Vahid Shahrezaei

Biological systems face constant fluctuations and perturbations, such as environmental changes or inherent stochasticity in their molecular processes, yet tend to produce robust and reliable behaviour. However, our knowledge on the mechanisms underlying biological robustness is still very limited. In this general area I have two projects of interests.

1. Turing has suggested basic models that can produce patterns in dynamics of reaction-diffusion systems. In this project, we use lattice based spatial stochastic simulations of chemical networks to study the robustness of such systems to noise in gene expression.

2. Among all multicellular organisms, Caenorhabditis elegans offers a unique experimental system to study robustness because of its remarkably reproducible development. The aim of this project is to reveal the extent of gene expression variability between phenotypically identical animals, as well as understand its attributes and functional implications. We have data from biologists in the developmental programs of this worm that we will combine with agent based simulations to unravel mechanisms of developmental robustness.

MSc projects with Dr Igor Shevchenko

- **Large scale low-frequecny variability of the midlatitude ocean circulation**
  Understanding origins of the large-scale low-frequency variability (LFV) of the ocean is not only one of the central questions in the Earth system modelling and geophysical fluid dynamics, but also one of the serious challenges in predictive understanding of climate change. The midlatitude atmosphere and ocean possess significant interannual variability and several large-scale variability modes on decadal and interdecadal timescales. Physical origins of the LFV modes remain unclear, and it is not even known to what extent these origins are intrinsic atmospheric, intrinsic oceanic, or coupled oceanic-atmospheric. This project focuses on studying the intrinsic oceanic LFV.

- **Absorbing boundary conditions for nonlinear wave equations**
  Many problems in science and engineering are naturally formulated in unbounded domains; typical examples originate from fluid dynamics, solid mechanics, aerodynamics, electrodynamics, acoustics, etc. However, numerical simulations of such problems require a finite computational region. This project is aimed to design absorbing boundary conditions for efficient and robust numerical simulations of nonlinear wave equations in unbounded domains.

- **Stochastic parameterisations for ocean models**
  Stochastic parameterisations of oceanic eddies play an important role in geophysical fluid dynamics because of their ability to represent complex physical processes with relatively simple models. In this project we develop parameterisations for the quasi-geostrophic model of wind-driven ocean gyres and analyse their efficiency in modelling unresolved scales.

- **Multiscale oceanic energetics**
  The goal of this project is to study inter-scale energy transfers in the ocean, examine the multi-scale nature of the forward and backward energy cascade, and how the energy transfers depend on viscosity.

- **Modelling the ocean with primitive equations**
  Modelling the ocean with primitive equations is a vast and active area of research in geophysics. The goal of this project is to simulate and study ocean currents in the North Atlantic with using the Regional Ocean Modelling System (ROMS).

- **Bifurcation analysis of dynamical systems with degenerative solutions**
  In this project we consider convection in a porous material saturated with fluid and heated from below. This problem belongs to the class of dynamical systems with nontrivial cosymmetry, which gives rise to a hidden parameter in the system and continuous families of infinitely many equilibria, and leads to non-trivial bifurcations. It is planned to study nonlinear phenomena resulting from the existence of cosymmetry, describe different non-classical bifurcations, and the selection scenarios (namely, which of infinitely many equilibria can be realized in physical experiments).

Approximations of stochastic dynamics

Supervisor: Dr Philipp Thomas (p.thomas@imperial.ac.uk)

Stochastic phenomena are widespread in biology, yet many interesting problems are not analytically tractable. In this project, you we will study the dynamics controlling the expression of genes in the cell through the Wentzel-Kramers-Brillouin (WKB) approximation. This approximation, derives from a path integral approach to the master equation, and allows to study the stochastic motion through an effective deterministic particle in a potential. Some basic knowledge of differential equations, stochastic processes and simulation is advantageous.

Literature:
Bressloff, Paul C (2014) *Stochastic Processes in Cell Biology.* Springer Book

Stochastic population dynamics in time-dependent environments

Supervisor: Dr Philipp Thomas (p.thomas@imperial.ac.uk)

Controlling the growth of cell populations is an important problem in biomedical applications. In this project, you will investigate solutions to age-structured population dynamics with time-dependent inputs such as stress or drug treatment. We will develop analytical solution methods for simple populations to quantify their asymptotic growth. Of particular interest will be to distinguish features of individuals in growing from dying populations (super-/subcritical processes) using the method of characteristics. Some basic knowledge of stochastic processes is advantageous but not necessary.

Literature:
Inaba, H (2017). *Age-structured population dynamics in demography and epidemiology.* Springer Book.

Bayesian inference of stochastic reaction networks

Supervisor: Dr Philipp Thomas (p.thomas@imperial.ac.uk)

Biochemical reactions occur stochastically in living cells. To reliably estimate the rates of these reactions, we need to take into account this stochasticity observed in vivo. Bayesian inference is often the preferred choice for this purpose, but it is computationally expensive because it requires sampling from the posterior distribution of parameters via MCMC. In this project, we will explore an alternative route to the inverse problem. The goal will be to use an asymptotic expansion of the stochastic process to infer the posterior distribution of system parameters.

Literature:
Fröhlich, F., Thomas, P., Kazeroonian, A., Theis, F. J., Grima, R., & Hasenauer, J. (2016). Inference for stochastic chemical kinetics using moment equations and system size expansion. *PLoS Computational Biology*, *12*(7), e1005030.
Thomas, P., & Grima, R. (2015). Approximate probability distributions of the master equation. *Physical Review E*, *92*(1), 012120.

Roll/streak/wave interaction in shear flows and turbulent spot formation – Dr A. Walton

In recent times a dynamical systems picture of laminar-turbulent has emerged in which equilibrium solutions of the Navier-Stokes equations play a key role in transition and turbulent dynamics. These equilibrium solutions consist of three crucial components: a roll flow in the cross-stream plane, a streamwise streak and a three-dimensional wave. These three components interact in a mutually sustaining manner in which the roll flow drives a spanwise-modulated streak which is itself unstable to the wave. The wave then self-interacts nonlinearly to reinforce and re-energize the roll flow. At high Reynolds number this interplay can be expressed in terms of an asymptotic theory known as **vortex-wave interaction**. It is possible to formulate and solve the interaction equations for a wide variety of viscous shear flows. In this project we concentrate on one of the well-known properties of the solution of such systems: the appearance of solutions which localize as the amplitude of the motion is increased. This **localization** is thought to be connected to the experimental observation that at relatively small disturbance levels viscous travelling waves cause an instability of the flow which leads to the formation of **turbulent spots**.

We propose to study the interaction between a roll, streak and viscous wave in an **asymptotic suction boundary layer**. It can be shown that the main part of such an interaction is governed by the nonlinear system:

$$\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \;\; v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = \frac{\partial^2 w}{\partial y^2},$$

subject to the boundary conditions

$$w = A\sin z, \;\; v = -1 \;\; \text{on}\, y = 0, \;\; w \to 0 \text{ as } y \to \infty.$$

Here (v, w) are the normal and spanwise components of the roll flow and the condition on w at the wall represents the wave forcing with amplitude A. It can be shown that this system has a nonlinear exact solution for small values of the spanwise coordinate z up to a critical amplitude for A. We propose to carry out numerical calculations of the full equations to investigate how the localization in the system is related to the singularity in the local exact solution.

References

Deguchi, K., Hall, P. & Walton, A. G. 2013 The emergence of localized vortex-wave interaction states in plane Couette flow. *J. Fluid Mech.* **721**, 58–85.

Dempsey, L.,J., Deguchi, K., Hall, P. & Walton, A. G. 2015 Localized vortex/Tollmien-Schlichting wave interaction states in plane Poiseuille flow. Preprint available on request.

Useful course to take: M4A30 Hydrodynamic stability.

Investigation of the stability properties of shear flows over compliant surfaces – Dr A. Walton

The behaviour of fluid flows over flexible surfaces is a challenging one for theoretical fluid dynamicists. The traditional instabilities one encounters over a rigid wall are supplemented by elasic modes arising from the response of the boundary.
In this project we will consider flows through channels with either one or both walls possessing compliant properties. The flow can be generated by applying a pressure gradient, moving the walls or a combination of both effects. A simple spring-backed plate model will be adopted to describe the motion of the boundary and we will assume that any perturbations of the surface are small, so that their effect on the basic flow will be a linear one. The aim of the project is to investigate the linear stability properties of the ensuing flow at high Reynolds number and/or at finite Reynolds number. The former analysis requires a knowledge of asymptotic methods, while the latter would involve computation with Matlab and require the student to write their own codes.

References:
P. G. Drazin: Introduction to Hydrodynamic Stability (C.U.P.)

Recommendation algorithms for implicit feedback with weighting (Dr Kevin Webster)

Recommender systems are frequently used in industry, and one broad categorisation of these algorithms is by the type of data. Explicit feedback data is when users have given specific ratings for items. Implicit data is data on user-item interactions (no explicit feedback) - this type of data is much more ubiquitous but not as directly usable. A popular algorithm for implicit data is the weighted matrix factorisation (WMF) algorithm. There are a few drawbacks to this algorithm that could be motivation for developing something different:

- Predictions of the model are not necessarily valid (without going into details, it is possible the model predicts values for a variable that are invalid). Can the model be cast into a probabilistic setting to treat this problem?

- It is not clear how to combine explicit and implicit feedback with this model

- Some applications require weighting recommendations according to certain criteria. Again it is not clear how this could/should be done with WMF

Prerequisites: some machine learning background (ideally in recommender systems), python

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Lyric trend analysis in popular music with NLP (Dr Kevin Webster)

Natural language processing is an important area of machine learning that has grown in prominence in applications where large amounts of natural language data is available. This project aims to apply these tools to identify patterns and trends in lyrics from a large and diverse corpus of popular music. Existing approaches for trend analysis or genre classification tend to focus on audio features, but relatively little work has been done on the analysis of lyrics. The structure and origin of this text corpus provides unique challenges in identifying relevant patterns to identify emerging trends over time, and the project will likely require to connect to a phonetic analysis of the corpus. This project would be a first step towards bringing the lyrics and audio together for a more complete treatment.

Prerequisites: some machine learning background (ideally with NLP), python, Tensorflow/PyTorch

Project supervisor: Dr Shahid Mughal, s.mughal@imperial.ac.uk
There is some considerable flexibility in the direction and scope of the projects and may well comprise aspects of theoretical analysis and computational work. Background in Fluid Dynamics, Asymptotic analysis and scientific computing (Matlab, Python, C or Fortran) would be most useful.

Project 1: Unsteady Fluctuations in a Compressible Uniform Steady Flow and Boundary-Layer Interactions.
Project supervisor: Dr Shahid Mughal, s.mughal@imperial.ac.uk

A number of research projects may be based on the general theme of modelling small fluctuations to the unsteady Navier-Stokes equations (NSEs) in a uniform compressible steady stream. The fluctuations may be due to acoustic, thermal and or turbulence related. Fluctuations in the environment are key components which give rise to or contribute to physical processes which lead to the generation of instabilities in a boundary-layer. Of particular interest is the issue of developing adequate models for free-stream turbulence, and or the related topic of how free-stream fluctuations (arising from say the wake of an aerofoil or turbulence grid in a wind-tunnel) subsequently become modified as the fluctuations convect along with the nominally steady uniform flow. How these free-stream fluctuations then initiate or interact with a developing boundary-layer and thus induce unsteady fluctuations in the boundary-layer is the concern.
Two projects are offered:

1. Free-stream turbulence modelling;

2. Compressible acoustic fluctuations.

References/Background material:
Hunt, J. C. R. & Graham, J. M. R. (1978). Free-stream turbulence near plane boundaries. J. Fluid Mech. 84 (2), 209-235.
Gulyaev, A. N., Kozlov, V. E., Kuznetsov, V. R., Mineev, B. I. & Sekundov, A. N. (1989) . Interaction of a laminar boundary layer with external disturbances. Fluid Dyn. 24(5), 700-710.
C. R. Illingworth, (1958). The effects of a sound wave on the compressible boundary layer on a flat plate. J. Fluid Mech. 3, 471.
P. W. Duck, (1990). The response of a laminar boundary layer in supersonic flow to small amplitude progressive waves. J. Fluid Mech. 219, 423-448.
Duck, P. W., Ruban, A. I. & Zhikharev, C. N. (1996). The generation of Tollmien-Schlichting waves by free-stream turbulence. J. Fluid Mech. 312, 341-371.

Project 2: Hypersonic Flow around a Blunted Slender Cone
Project supervisor: Dr Shahid Mughal, s.mughal@imperial.ac.uk

There is considerable interest in aerodynamic surfaces travelling very fast at Hypersonic speeds presently and will be even more so in the future. A common issue in such speed regimes is the existence of shocks and bluntness of the nose sections of bodies of revolution. The project will explore the effects of slenderness and bluntness in the inviscid and/or viscous flow regimes behind the shock. A combination of asymptotic and numerical approaches could be pursued.
References/Background material:
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Pressure-driven viscoelastic flows in channels with superhydrophobic wall structurings

Supervisors: Prof. D.T. Papageorgiou, Dr. P. Ray

Project Description.

Viscous fluids are hard to flow in micro geometries - very large pressure are required to generate useful flow rates. Such engineering design barriers become centrally important in modern microfluidics applications where the quest is to do engineering on the micro- and nano-scale, for example to build sub-millimeter lab-on-chip devices to do fast and cheap biosample analyses as well as contaminant testing for security applications.

One solution is to structure the walls of the device or channel to include grooves that contain gas and which can support the liquid meniscus thus reducing the liquid-solid contact area where drag is highest due to no-slip shear, and producing “lubricated" flows with desirable properties. Such devices are also used in cooling systems for commercial computer server applications - a schematic that illustrates the geometry and the flow is included here.

In many applications the fluids are not Newtonian but instead have elastic properties with the viscosity depending on the local shear rate. Different canonical models have been used in the literature and for the purposes of this project we will concentrate on two models: (i) a simpler *power law* non-Newtonian fluid, and (ii) the so-called Giesekus model. Both of these are appropriate for the structured surface flows we wish to study. The particular application we have in mind is in the use of such devices for blood oxygenation processes - during invasive operations (e.g. heart surgery) the blood stream is diverted outside the body where it needs to be kept oxygenated before it is re-introduced. Detrimental infections can occur when red blood cells come into direct contact at high shear with device walls, and we suggest to overcome such difficulties by using structured superhydrophobic surfaces that achieve drag reduction as well as smaller area contact. Blood is a viscoelastic fluid and hence the models proposed are appropriate.

Regarding the mathematical modeling, analysis and computations, these will evolve along the following lines:

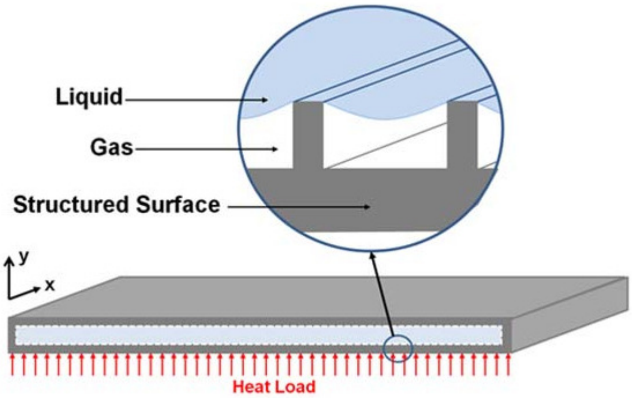

Figure 1: Schematic of a superhydrophobic channel used in heat enhancement applications. The flow is into the paper parallel to the direction of the grooves.

- Learn about viscoelastic fluids and how the Navier-Stokes equations are extended to deal with these problems.
- Develop the mathematical models for pressure-driven flow in channels with longitudinal gas-containing grooves. The liquid will be in the *Cassie state*, i.e. the liquid will entrap the gas pockets and flow over them. Initially we can assume that the interface is flat.
- Carry out a local analysis to describe the stress singularity at the liquid/gas/solid triple contact point. This will be guided by analogous work on the Newtonian problem.
- Construct numerical methods to compute the flow (e.g. finite-difference or finite-element) and produce results that will describe how the wall structuring influences effective slip. This will be done for the power law and Giesekus models.

Learning Outcomes. Several learning outcomes are anticipated, which are associated with:

- Complex fluids and the models used in non-Newtonian fluid dynamics.
- Microhydrodynamics and flows over superhydrophobic surfaces.
- Analysis of stress singularities in non-Newtonian flows.
- Numerical computations of Newtonian and non-Newtonian flows in channels with longitudinal grooves. These are typically elliptic two-dimensional problems.

Relevant courses. The following courses (or equivalent) from the Applied Mathematics M.Sc. program could prove useful, however not all of them are essential: Fluid Dynamics I, Fluid Dynamics II, Hydrodynamic Stability, Numerical Solution of Ordinary Differential Equations, Computational Partial Differential Equations, Asymptotic Analysis, Introduction to Partial Differential Equations.

References:

[1] E. Lauga and H.A. Stone. *Effective slip in pressure-driven Stokes flow*, J. Fluid Mech. **489**, 55–77, 2003.
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Nonlinear Partial Differential Equation (PDE) Studies Arising in Multilayer Flows

Supervisors: Prof. D.T. Papageorgiou

Project Description.

Immiscible multilayer flows are moving boundary problems encountered in numerous applications. The paradigm problem of a moving (or free) boundary problem is that of water waves - the free surface evolves spatiotemporally and must be determined as part of the solution. Multilayer problems that arise in industrial applications are typically viscous and involve more than one interface, e.g. the coating of a component by three immiscible fluids involves two internal interfaces and a free surface. Mathematically, we need to solve the Navier-Stokes equations in moving domains and in the process determine the domains themselves. The boundary conditions at interfaces are nonlinear and typically stiff - they contain high order spatial derivatives (e.g. surface tension provides 4 spatial derivatives).

This project is concerned with classes of PDEs that have been derived and partially studied for three-layer flows in pressure-driven channel flows [1, 2, 3]. There are two interfaces involved which gives rise to a coupled system on nonlinear PDEs that can be 4th order in space. The interesting aspect of the models is that their nonlinearities support a change of type from hyperbolic to elliptic (the overall system is parabolic of course) and such equations produce a host of interesting, and in many cases unexpected, dynamics. For example, different nonlinearities can produce bounded solutions, but small changes produce unbounded finite-time blow up.

The project will consider new computations and analysis where feasible, of such model equations. Possible directions are: (i) Homotopy type computations that revert from one stem to another as a parameter is varied, along with identification of general classes of flux functions that give rise to finite time blow up; (ii) Construction of heteroclinic traveling waves and their stability, with emphasis on the possibility of connecting states where the flux function is hyperbolic to ones where it is elliptic - such solutions, if they exist, would be novel as far as I know; (iii) extensions to additional physics (e.g. viscoelastic flows, electrified flows, flows under magnetic fields) to obtain richer classes of equations to study.

Prerequisites Students interested in this project should have a good knowledge of fluid dynamics, analytical and computational PDEs and interest in scientific computing.

References

[1] Papaefthymiou, E.S., Papageorgiou, D.T. and Pavliotis, G.A. 2013 Nonlinear interfacial dynamics in multilayer channel flows, *J. Fluid Mech.*, Vol. 734, pp. 114–143.
[2] Papaefthymiou, E.S. and Papageorgiou, D.T. 2015 Vanishing viscosity limits of mixed hyperbolic-elliptic systems arising in multilayer channel flows, *Nonlinearity*, Vol. 28, pp. 1607–1631.
[3] Papageorgiou, D.T. and Papaefthymiou, E.S. 2017 Nonlinear stability in three-layer channel flows, *J. Fluid Mech.*, Vol. 829, R2, doi:10.1017/jfm.2017.605.

Modelling of a chain fountain (Prof Degond)

This project is motivated by a recent experiment popularized by science blogger Steve Mould [1]. If the end of a long bead chain held in a container at a certain distance from the floor is pulled out of the container down to the floor, the chain leaps from the container above it, turning it into a chain fountain. While qualitative physical explanations of this phenomena have been given [2], no theory nor simulations have been provided for the dynamics of the chain. In particular, in the videos, beyond the spectacular fountain phenomenon, one observes that the chain is subject to oscillations and waves. The goal of the project is to study a continuum model of the chain previously derived [3]. In particular, we wish to provide a theoretical foundation of the heuristic derivation of the model, to provide adequate boundary conditions that can reproduce the fountain phenomenon and to study the resulting model both theoretically and numerically, ultimately providing a explanatory numerical model for the chain fountain phenomenon.
The model involves an interesting nonlinear coupling between a wave equation for the local tangential direction to the chain with an elliptic equation for the tension of the chain. Connections with classical mechanical model such as the slender rod model will be sought. Extension of the model to higher dimensions, to model e.g. the motion of a piece of cloth, can also be envisioned.

Supervisor: Pierre Degond (pdegond@imperial.ac.uk), in collaboration with P. Noble (Institut de Mathematiques de Toulouse (Pascal.Noble@math.univ-toulouse.fr).

References

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Professor Mauricio Barahona

MSc in Applied Mathematics

General topics:

Dynamics and graph theory. Network analysis.

Graph-based deep learning and inference.

Stochastic processes on graphs.

Dimensionality reduction, geometric projections of high-dimensional data.

Community detection on graphs.

Optimisation.

Areas of application: General data science, social networks, biomathematics and healthcare applications.

Some examples of areas and projects:

Title: Theory of graph-based data analysis: conceptual and mathematical extensions of techniques for the representation of data as graphs, and the coarse-graining of such representations.

Some possible mathematical topics include:

* time-varying networks and their partitions: statistical detection of break points using Gaussian processes

* representations of data through graphs: geometric, sparse optimal graphs that preserve structural and spectral properties of data

* multiplex graphs and spectral characterisation of graph alignment

* relation of community detection in graphs and Krylov methods

* simplicial complexes to represent data structures

* generalised Kirchoff indices in graphs: graph robustness, centralities, and escape times.

Title: Text as high-dimensional data: extracting topics from document corpora

Application of recently developed techniques in our group for the analysis of high dimensional data using graph theoretical techniques linked to geometric constructions, as well as the use of diffusion dynamics on graphs for community detection.

Application to the analysis of text using Doc2Vec, unsupervised graph partitioning, and supervised label classification. Datasets include either healthcare reports or financial reports.

With collaborators in the NHS or the Finance Group in the Business School.

Title: Extracting the landscape of cellular evolution from high-dimensional transcriptomics data of stem cell development.

Haematopoietic stem cells (HSC) are a very rare population of cells responsible for sustaining blood production throughout life. HSCs reside in specialized niches in bone marrow, which beyond physical support regulate fundamental stem cell processes including proliferation, self-renewal and multilineage differentiation. The HSC niche is a complex multi-cellular entity composed of different types of endothelial and mesenchymal cells. Importantly, recent single cell transcriptomic studies revealed a previously unappreciated high level of cellular heterogeneity in the niche. Yet, the exact cells that constitute the HSC niche, how they regulate HSC function and the functional relevance of this high heterogeneity are still largely unknown. We will use these recently published single cell RNA sequencing data sets to map the expression of critical HSC maintenance factors to distinct niche cell populations and, investigate the hierarchical relationship between distinct sub-populations of endothelial and mesenchymal cells.

This analysis will be carried out by using dimensionality reduction techniques that respect the temporal progression of the cellular state using similarities based on Gaussian Processes and similarity graphs to extract meaningful coordinates for cell differentiation and sub-populations of niche cells with a role in regulating HSC function in response to induced-stress haematopoiesis using specific markers.

Title: Graph-based deep learning: Bringing together graphs, stochastic processes on graphs and deep neural networks.

Recently, extensions of deep learning algorithms have been successfully applied on datasets encoded in graphs (Graph convolutional neural networks). We have developed a method to solve such semi-supervised learning problems without deep neuronal architectures, but with similar classification accuracy using diffusive processes. Several projects exist in this area from the classification of networks based on high-dimensional features to developing state-space recurrent neural network models that combine the interpretability of Hidden Markov models with high predictability of deep learning architectures.

Applications to citation networks on documents, brain networks, time series, and patient trajectories.

With Dr Rob Peach

Title: Identifying Naturally Occurring Relationships Between Hospitals and Communities in England

Objective: To examine naturally occurring catchment areas for hospitals in England and compare these to the embedded administrative structure of the NHS.
Data: Hospital Episode Statistics data for patients with chronic disease in England from 2016-18.
Specific Aims:

- Use Markov Multiscale Community Detection to construct catchment areas for hospitals providing care to patients with chronic disease in England.
- Compare results to existing methods used to define catchment areas.
- Quantify the similarity of catchment areas to existing administrative boundaries in the NHS.
- Identify regions of discrepancy with current boundaries and examine the implications of this discrepancy for patient outcomes.

With Dr J Clarke

Title: Inferring and predicting probabilistic patterns in pathways of care

Supervisors: Dr Sam Greenbury, Dr Elsa Angelini, Prof Mauricio Barahona (Department of Mathematics, EPSRC Centre for Mathematics of Precision Healthcare and ITMAT Data Science Group)

Description:

HyperTraPS (Hypercubic Transition Path Sampling) is a recent approach for performing efficient Bayesian inference describing the acquisition or loss of features in a binary state space [1, 2].

Given data exhibiting the presence or absence of such features, combined with assumptions for the dynamics of how they may be gained or lost, powerful predictive models can be inferred for describing dynamics. The application of such models ranges from disease and evolution to care pathways in healthcare.

However, a wide range of mathematical advances are possible, for example: (1) understanding inference where the features can be both gained and lost or when data has been censored; (2) Where the underlying data is potentially made up of a mixture of signals, methods for distinguishing such signals or subtypes is of great value for stratification.

This project will develop and apply HyperTraPS to model pathways of care in new-borns admitted to neonatal care units, utilising machine learning ready 'big data' from the National Neonatal Research Database [3] with the aim of translatable insights.

Prerequisites:

knowledge and interest in Bayesian inference, Markov models/processes, python, machine learning/data science methods

References:

[1] HyperTraPS: Inferring probabilistic patterns of trait acquisition in evolutionary and disease progression pathways' by Sam F. Greenbury, Mauricio Barahona and Iain G. Johnston, Cell Systems 2019, https://doi.org/10.1016/j.cels.2019.10.009

[2] https://www.imperial.ac.uk/news/193946/new-maths-reveals-diseases-progress-drugs/

[3] https://www.imperial.ac.uk/neonatal-data-analysis-unit/neonatal-data/utilising-the-nnrd/

Title: Novel methods for outlier detection in healthcare data

Supervisors: Dr Sam Greenbury, Dr Elsa Angelini, Prof Mauricio Barahona (Department of Mathematics, EPSRC Centre for Mathematics of Precision Healthcare and ITMAT Data Science Group)

Description:

Identifying data that lies outside expected variation is of crucial importance across myriad fields. In healthcare, for example, it is vital at several levels from correcting data entry to monitoring good clinical practice to alerting clinicians to abnormal physiological signals in patients. This project aims to develop novel approaches for identification of anomalous patterns in neonatal care. Current approaches are based upon standard statistical tests where more sophisticated methods are now potentially available.

The project is open-ended in exploration of such alternative approaches: supervised machine learning (SVMs, Random Forests or deep learning approaches) and unsupervised methods such as Bayesian models or graph theoretical representations may be used to identify rare patterns.

In addition to the value of developing such new methodologies for outlier detection across all fields, findings have the potential for direct translation in this project for measuring the quality of care provided to neonates across the population utilising cleaned 'big data' [1].

Prerequisites: knowledge and interest in outlier/anomaly detection, machine learning/data science methods, python

References:

[1] https://www.imperial.ac.uk/neonatal-data-analysis-unit/neonatal-data/utilising-the-nnrd/

Title: Unsupervised classification of cancer progressions

Supervisors:

Dr Sam Greenbury and Prof Mauricio Barahona (Department of Mathematics and EPSRC Centre for Mathematics of Precision Healthcare)

Description:

Inferring the order of genetic and physiological changes is one of the central approaches to understanding the way cancer progresses, providing a means for prevention and treatment. A progression may be considered as a partially ordered set of events. From collected data, some methods aim to infer such partially ordered sets, while others consider pathways in the underlying state space. Both approaches lead to progressions that may be abstractly characterised as sequences of symbols. In this project, you will investigate methods for performing unsupervised classification of such sequences. This will involve finding and developing appropriate distance metrics for the problem and using machine learning methods in order to detect and characterise common patterns, with the aim of uncovering previously undetected pathways from real data.

Prerequisites:

knowledge of Bayesian inference/networks, Markovian dynamics, python, basic machine learning methods.
