Applied Mathematics Projects 2022 - 2023

Imperial College London

Projects with Dr Ryan Barnett

1. **Phonons in an expanding or contracting BEC**

   In quantum mechanics, any particle can be classified either as a fermion or a boson. When a collection of bosons is cooled to a sufficiently low temperature, an exotic state of matter called a Bose-Einstein condensate (BEC) is formed. Since its realisation in 1995 (for a good pedagogical review see [1]), BEC has proven to be a fertile ground for applications in quantum simulations. For example, they can provide clean realisations of toy models used to understand disparate physical systems.

   The low-energy excitations in BECs are often called phonons and are similar (though sometimes superficially) to vibrational modes of a crystal or sound waves in air. In this project, we will investigate such collective excitations of a BEC that is *expanding* or *contracting*. Experiments along these lines have recently been carried in [2] and have strong analogies with certain cosmological models. We will attempt to understand the puzzles found in these experiments using quantum field theory methods of many-particle systems.

   [1] A. J. Leggett, *Bose-Einstein condensation in the alkali gases: Some fundamental concepts*, Rev. Mod. Phys. 73, 307

   [2] S. Banik, M. Gutierrez Galan, H. Sosa-Martinez, M. Anderson, S. Eckel, I. B. Spielman, G. K. Campbell, *Hubble Attenuation and Amplification in Expanding and Contracting Cold-Atom Universes* arXiv:2107.08097

2. **Exotic states in rotating condensates**

   Diagonalising the Hamiltonian corresponding to a charged particle confined to a plane with a constant perpendicular magnetic field is one of the canonical problems in quantum mechanics. The resulting spectrum has a fascinating feature: there are (typically) large degeneracies associated with each eigenenergy. Such collections of degenerate states are called Landau levels, and the one with lowest energy is called the lowest Landau level (LLL). These large degeneracies play an essential role in (fractional) quantum Hall systems [3].

   Systems of bosons in the LLL have been experimentally explored much less, partially due to the fact that most bosons used the lab are neutral (i.e. they carry no charge). For such systems, a magnetic field (as experienced by charged particles) can be mimicked by mechanically rotating the system. Recent experiments have reached the LLL regime using such rotation with the additional technical trick of geometrical squeezing [4]. In these experiments a bosonic crystalline phase was observed.

   This project will aim to understand this experiment using the method of exact diagonalisation.

   [3] R. B. Laughlin, *Fractional quantization*, Rev. Mod. Phys. 71, 863 (1999)

   [4] Biswaroop Mukherjee, Airlia Shaffer, Parth B. Patel, Zhenjie Yan, Cedric C. Wilson, Valentin Crépel, Richard J. Fletcher, Martin Zwierlein, *Crystallization of Bosonic Quantum*

Hall States, arXiv:2106.11300

3. **Other**

   I am happy to discuss other project ideas of mutual interest. Projects that are deviations of the above two specific directions can be considered as well. I prefer working with students who have (or are obtaining) experience in quantum mechanics.

Dynamics of Active Fluids: an exploration of the Toner-Tu equation

Supervisor: Thibault Bertrand

Description

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.

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].

Plan

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 analytical side, we will perform linear stability analysis over the equations of motion to determine the stability of certain phases. On the numerical side, we will develop methods to numerically solve the Toner-Tu equation and compare the results to our theoretical predictions [11]. These methods may include: finite differences and spectral methods which were hugely successful in classical hydrodynamics.

Prerequisites: Good coding skills are essential. Familiarity with partial differential equations and/or fluid dynamics is desirable.

References

[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):9598, 2013.

[3] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck. Phys. Rev. Lett., 110:238301, 2013.

[4] S. Henkes, Y. Fily, and M. C. Marchetti. Phys. Rev. E, 84:040301, 2011.

[5] G. K. Batchelor. An Introduction to Fluid Dynamics. Cambridge University Press, 1967.

[6] J. Toner and Y. Tu. Phys. Rev. Lett. 75, 4326, 1995.

[7] J. Toner and Y. Tu. Phys. Rev. E 58, 4828, 1998.

[8] J. Toner, Y. Tu, S. Ramaswamy. Annals of Physics, 318, 170244, 2005.

[9] S. Ramaswamy. Ann. Rev. Cond. Mat. Phys., 1, 323-345, 2010.

[10] M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, Madan Rao, and R. Aditi Simha. Rev. Mod. Phys. 85, 1143, 2013.

[11] J. Dunkel, S. Heidenreich, K. Drescher, H. H. Wensink, M. Br, R. E. Goldstein. Phys. Rev. Lett., 110, 228102 (2013)

Behaviour of active filaments in crowded environments

Supervisor: Thibault Bertrand

Description

Understanding the dynamics of biological agents in porous media is of prime importance. Indeed, it has vast applications in biology, medicine and industry [1, 2]. Examples include myxobacteria gliding in soils, the dynamics of engineered bacteria in tumor environments, and bacteria-based water purification and decontamination in the ground. Initial studies have shown that the dynamics of these biological agents in crowded environments highly depends on their shape, their size and the environmental properties such as the porosity, permeability etc.

From a theoretical point of view, many such biological agents can be thought of as active polymer chains, whose length and the stiffness is dependent on the species under consideration. In recent years, there has been huge research interest in the study of active polymers; existing models usually describe these active polymers a beadstrings in which each bead (or monomer) is subject to both thermal fluctuations but also an active force (or self-propulsion). Two strategies have been considered to model this active forcing: (i) the active force on each monomer can be applied in a random direction subject to rotational diffusion *or* (ii) the active force can be applied tangentially to chain. These two different conventions have been shown to lead to very different structural properties. The first kind of chain undergoes shrinkage followed by swelling of the structure with active forces [3], whereas the tangentially driven chain has been shown to form spirals and undergo snake-like motion transiently [4].

While the behavior of passive polymer chains in porous media has been well-studied, the behavior of active filaments in crowded environments remains mostly unexplored [5] with the notable exception of a recent study showing that stiffness of active filaments promote their efficient transport in two-dimensional porous media [6]. While flexible chains curl up and tend to get trapped when they form spirals, the motion of stiff active polymers is almost unhindered by the obstacles in the porous medium.

Plan

The project will try to answer a number of interesting questions. Our main aim is to understand the dynamics of active polymers and focus on the competition between knotting/entanglement of the filaments and the transport of filaments in two situations: (i) in free space and (ii) in model porous media made of arrays of obstacles. To do so, we will develop and analyse computer simulations.

After an initial review of the literature on the subject, you will develop numerical simulations which you will compare to existing results. We will then extend the existing literature by exploring numerically a variety of conditions. Our numerical results will be interpreted in the framework of existing theories for active matter and transport in crowded environments.

Prerequisites: Good coding skills in the programming language of your choice is essential (recommended programming languages: C/C++, matlab or python). Existing codes can be provided as starting point.

References

[1] T. Bhattacharjee and S. S. Datta. Nature Communications 10, 2075, 2019.

[2] T. Bhattacharjee and S. S. Datta. Soft Matter 15, 9920-9930, 2019.

[3] A. Kaiser, S. Babel, B. ten Hagen, C. von Ferber and H. Löwen. J. Chem. Phys. 142, 124905, 2015.

[4] R. E. Isele-Holder, J. Elgeti and G. Gompper. Soft Matter, 11, 7181-7190, 2015.

[5] B. Chakrabarti, C. Gaillard and D. Saintillan. Soft Matter, 16, 5534-5544, 2020.

[6] Z. Mokhtari and A. Zippelius. Phys. Rev. Lett., 123, 028001, 2019.

Transport of micro-organisms in complex environments

Supervisor: Thibault Bertrand

Description

Micro-organisms, like bacteria, generically explore complex environments (like soils for instance) to find nutrients. Over the past two decades, active matter has shown to be an avenue for a quantitative description of complex biological processes. Yet, active particles models remain relatively minimal and our understanding of their transport in complex environments is lacking. Further, understanding the optimization of exploration strategies of immune cells in complex environments has relevance to the immune response for instance.

To approach real-life settings, it is thus interesting to study the effect of interactions of active particles (e.g. cells, bacteria ...) with their environment (e.g. external forcing, obstacles ...). In these complex environments, randomness and crowding can either enhance or limit the efficiency of biological or artificial systems performing complex tasks (e.g. finding nutrients or finding infected cells).

Classical active particle models include run-and-tumble particles, active Brownian particles and active Ornstein-Uhlenbeck particles [1]. The group has previously studied the effect of physical obstacles on single run-and-tumble particle dynamics, showing the existence of an optimal diffusivity function of the particle tumbling rate and the obstacle density and thus, the possibility for a run-and-tumble particle to enhance its exploratory capabilities by tuning its tumbling probability [2].

Moreover, bacteria like *E. Coli* are known to adjust their behavior in order to navigate to regions of highest nutrient concentration; this is called chemotaxis. In particular, *E. Coli* was shown to modulate their tumbling rate in reaction to nutrient concentration gradients. The exact details of its chemotactic strategy are yet unknown but can be introduced to a certain degree in minimal mathematical models [3].

Plan

Building upon the existing active particle models, we will study the dynamics of active particles by means of simulations and analytical methods in complex (potentially time-varying) environments with physical obstacles and passive forcing (e.g. chemical gradients). We may start by considering environments with spatially dependent nutrient concentrations. We will then consider environments with physical obstacles as well. We will characterize the particle trajectories and quantify their exploratory efficiency studying the trade-off between gradient climbing and exploration on the effective diffusion of the particles in environments with obstacles. We will compare different active particle models and study the influence of the obstacles shape on trapping and escape of active particles [4,5]. Finally, if time permits, we will consider different obstacle geometries and may study whether *E. Coli* is any good at exploring a maze.

Prerequisites: Good coding skills in the programming language of your choice is essential (recommended programming languages: C/C++, matlab or python).

References

[1] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe. Active particles in complex and crowded environments. Rev. Mod. Phys., 88:045006, 2016.

[2] T. Bertrand, Y. Zhao, O. Bénichou, J. Tailleur, and R. Voituriez. Optimized diffusion of run-and-tumble particles in crowded environments. Phys. Rev. Lett., 120:198103, 2018.

[3] H. C. Berg. E. coli in Motion. Springer, 2004.

[4] A. Guidobaldi, Y. Jeyaram, I. Berdakin, V. V. Moshchalkov, C. A. Condat, V. I. Marconi, L. Giojalas, and A. V. Silhanek. Geometrical guidance and trapping transition of human sperm cells. Phys. Rev. E, 89:032720, 2014.

[5] M. Souzy, A. Allard, J.-F. Louf, M. Contino, I. Tuval, and M. Polin. Microbial narrow-escape is facilitated by wall interactions. Phys. Rev. Research, 4:L022029, 2022.

Dynamics of disordered active solids

Supervisor: Thibault Bertrand

Description

Active solids (or elastic active matter) consists of self-propelled particles embedded in an elastic matrix. In active solids, there is an interesting competition between the shape-preserving property of the elastic matrix (a solid resists deformation) and the non-equilibrium nature of the active particles embedded in the matrix. This gives active solids incredibly interesting mechanical and dynamical properties not seen in common passive solids. For instance, it was recently reported that active solids can develop odd elasticity [1,2], display autonomous waves and global motion [3] as well as emergent synchronization of its active components [4,5,6].

An elastic solid can be modelled as a network of mass-springs systems. Up to now, studies of active solids have focused on networks of springs with crystalline order (hexagonal lattices for instance). These networks of springs are inherently hyperstatic; they have more constraints than degrees of freedom. However, disordered solids (like jammed solids) in the connectivity of the network is tuned to reach isostaticity have been shown to display very different vibrational and mechanical properties to that of crystalline solids. Combining disorder, non-reciprocal interactions and activity in elastic solids may lead to a rich new phenomenology.

Plan

Building upon the existing studies, we will model disordered networks of active Brownian particles linked by linear springs. We will study how disorder may affect the synchronization between the active constistuents of our active solids. We will also introduce non-reciprocal interactions breaking the principle of action-reaction for each of the links on the network and study the emergent mechanical properties of the solid. This project will involve simple numerical simulations as well as analytics for instance using effective medium theory.

Prerequisites: Good coding skills in the programming language of your choice is desirable (recommended programming languages: C/C++, matlab or python).

References

[1] M. Fruchart, C. Sheibner, and V. Vitelli. arXiv:2207.00071, 2022.

[2] C. Scheibner, A. Souslov, D. Banerjee, P. Surowka, W. T. M. Irvine, and V. Vitelli. Nature Physics 16, 475-480, 2020.

[3] H. Xu, Y. Huang , R. Zhang, and Y. Wu. arXiv:2208.09664, 2022.

[4] E. Ferrante, A. E. Turgut, M. Dorigo, and Cristián Huepe. New J. Phys. 15, 095011, 2013.

[5] J. Binysh and A. Souslov. Nature Physics 18, 1142-1143, 2022.

[6] P. Baconnier, D. Shohat, C. Hernández López, C. Coulais, V. Démery, G. Düring, and O. Dauchot. Nature Physics 18, 1234-1239, 2022.

Project with Dr Borovykh, Anastasia

Optimal datapoint selection for machine learning

Deep neural networks are able to achieve excellent performance when trained on big datasets, even if the input data size is very large (e.g. 28x28 pixels for the MNIST dataset). One explanation for their good performance in high dimensions is that the data lies in a latent space with much lower dimensionality than that of the full data encoding space. Large datasets, potentially in combination with the implicit bias that occurs during training, can then be seen as a reasonable way of learning robust representations. The size of the dataset however clearly impacts the training efficiency. System constraints such as on-device computing or simply the fact that large datasets are not always available has led to a renewed interest in learning over small datasets. A challenge with using small datasets is that it is not clear that the critical characteristics of a function will be captured. While augmenting a small dataset is an option when a large datasets is not available, other approaches have focused on defining and obtaining `good' datapoints for which the learning can be efficient and lead to a robust representation. Also in the literature on interpolators and mesh optimization schemes interesting approaches for choosing relevant datapoints have been presented. Typically, this amounts to selecting points in `critical' areas of the function based on \eg the curvature. In this project we will compare the performance of machine learning over large and distilled datasets, where the distilled datasets are created by choosing optimal points according to different criteria, specifically, information-theoretic, coresets, sensitivity and curvature-based criteria. The machine learning methods we will consider are neural networks, kernel methods, Gaussian processes.

References:

- Boyan Bonev, Feature selection based on information theory, 2010
- Michael Garland and Paul S Heckbert. Surface simplification using quadric error metrics. In Proceedings of the 24th annual conference on Computer graphics and interactive techniques, pages 209–216, 1997
- Myunggwon Hwang, Yuna Jeong, and Wonkyung Sung. Data distribution search to select core-set for machine learning. In The 9th International Conference on Smart Media and Applications, pages 172–176, 2020
- Mansheej Paul, Surya Ganguli, and Gintare Karolina Dziugaite. Deep learning on a data diet: Finding important examples early in training. Advances in Neural Information Processing Systems, 34:20596–20607, 2021

Project with Dr Borovykh, Anastasia

Training of spiking neural networks with interacting particle optimisers

The amount of computational power required to run top performing deep learning models has increased at a rate of 10x per year from 2012 to 2019 [1]. A new generation of brain-inspired spiking neural networks (SNNs) has shown promising results in improving the energy efficiency of machine learning. In SNNs neurons interact via spikes: instead of passing the weighted sum from the previous layer through a sigmoid or ReLU nonlinearity, the weighted sum contributes to the membrane potential of the neuron. Only if the membrane potential reaches a certain threshold dose the neuron transmit information to its subsequent connections. Most neuronal inputs are spikes of very short bursts of electrical activity. The expected efficiency gain comes from the fact that the neurons will be at rest most of the time and a sparse data structure is more efficient to store. However, training SNNs is complicated by the discontinuities introduced by the spikes and the application of gradient-based learning is not trivial. In this project we will begin with a literature review of the state-of-the-art methodologies for training SNNs to better understand their positives and negatives. Then we will explore the use of gradient-free interacting particle-based optimisers to optimise the parameters of the spiking neural network.

References:

- Eshraghian, Jason K., et al. "Training spiking neural networks using lessons from deep learning." arXiv preprint arXiv:2109.12894 (2021)
- [1] Neil C Thompson, Kristjan Greenewald, Keeheon Lee, and Gabriel F Manso. The computational limits of deep learning. arXiv preprint arXiv:2007.05558, 2020
- Borovykh, Anastasia, et al. "On stochastic mirror descent with interacting particles: convergence properties and variance reduction." Physica D: Nonlinear Phenomena 418 (2021): 132844

A mathematical model of tumour-immune interactions

Supervisor: Barbara Bravi (Department of Mathematics, Imperial College London)
Collaborator: Eszter Lakatos (Chalmers University of Technology, Gothenburg)

For the immune system to control cancer, protein fragments carrying cancer-related alterations, neoantigens, have to be presented on cancer cells to be recognized by immune cells (T cells) via a specific binding to their surface receptors. Neoantigens are currently highly sought-after targets for immunotherapy design, however many open questions need to be answered to develop neoantigen-based immunotherapies of clinical utility. It is indeed extremely difficult to predict what neoantigens are immunogenic (i.e., can trigger an immune response) and what factors of the tumour immune microenvironment contribute to a durable and robust immune response against cancer.

Mathematical models and simulations can be extremely helpful to shed light on these open questions [1], and the aim of this project is to develop a new mathematical approach to this problem. We will appeal to existing formulations of the interacting dynamics of cancer and T cells [2] but we will include specific information on the molecular composition of neoantigens and T cell receptors that is becoming available through high-throughput sequencing experiments. The project will involve the following steps: *(i)* to determine a neoantigen-receptor interaction matrix that incorporates information on the molecular binding between neoantigens and receptors by applying recent machine learning methods developed for this task [3]; *(ii)* to solve numerically the dynamics induced by such interactions to study different scenarios depending on the predicted binding strength, the population density of cancer and T cells, as well as their phenotypic diversity.

This project is in collaboration with Dr. Eszter Lakatos at Chalmers University of Technology, Gothenburg.

References

1. Lakatos E, Williams MJ, Schenck RO, Cross WCH, Household J, Zapata L, et al. Evolutionary Dynamics of Neoantigens in Growing Tumors. Nature Genetics. 2020;52(10):1057–1066.
2. Almeida L, Audebert C, Leschiera E, Lorenzi T. Discrete and Continuum Models for the Coevolutionary Dynamics between CD8+ Cytotoxic T Lymphocytes and Tumour Cells. arXiv; 2021.
3. Weber A, Born J, Rodriguez Martínez M. TITAN: T-cell Receptor Specificity Prediction with Bimodal Attention Networks. Bioinformatics. 2021;37(Supplement_1):i237–i244.

Interacting Genomic Informational Field Theory

Supervisor: Barbara Bravi (Department of Mathematics, Imperial College London)
Collaborator: Cyril Rauch (Department of Veterinary Medicine & Science, University of Nottingham)

It is extremely complex to analyse all gene effects involved in phenotypic traits, as a consequence, current methods of genotype-phenotype associations are often limited to the determination of leading or average contributions. A new method, inspired by field theory in physics and called genomic informational field theory (GIFT), has been recently proposed [1], which is able to leverage extensively the information of genetic distribution density functions underlying a given genotype-phenotype mapping.

However, GIFT does not include the effect of gene interactions in the phenotypic distribution. Gene knock-out experiments have revealed an extensive pleiotropy, that is, many genes are simultaneously associated to a certain phenotypic effect and, by interacting, they confer robustness to its expression. The aim of this project is to develop a gene-interacting version of GIFT. We will appeal to drift-diffusion processes with defined boundary conditions and to their path formulation [2–4] to, first, fully write down the equations describing interacting GIFT. Next, the project will involve the numerical exploration of the stochastic solution (starting from the linear interaction regime) to determine what interaction and parameter regimes produce the observed robustness of the genotype-phenotype mapping.

The project is in collaboration with Dr. Cyril Rauch at the university of Nottingham.

References

1. Rauch C, Kyratzi P, Blott S, Bray S, Wattis J. GIFT: New Method for the Genetic Analysis of Small Gene Effects Involving Small Sample Sizes. Physical Biology. 2022;20(1):016001.
2. Wang S, Venkatesh A, Ramkrishna D, Narsimhan V. Brownian Bridges for Stochastic Chemical Processes—An Approximation Method Based on the Asymptotic Behavior of the Backward Fokker–Planck Equation. The Journal of Chemical Physics. 2022;156(18):184108.
3. Hertz JA, Roudi Y, Sollich P. Path Integral Methods for the Dynamics of Stochastic and Disordered Systems. J Phys A: Math Theor. 2017;50:033001.
4. Yasuda K, Ishimoto K. Most Probable Path of an Active Brownian Particle. arXiv; 2022.

Electrowetting: Analysis of the Triple Contact Point

Dr Sam Brzezicki

This project uses complex variable methods to both find and analyze the behaviour of solutions to electrostatic problems in electrowetting applications, in particular in close proximity to the so-called triple contact point.

Electrowetting is the process of changing the wetting properties of a surface by applying an electric field. In this project we will be interested in studying a static charged droplet at rest on a substrate with an applied electric field. The angle that the droplet makes with the substrate, known as the contact angle, has been widely investigated and the nature of solutions near this point at which the substrate, background medium and droplet all meet, known as the triple contact point (or triple contact line) is of great interest. This project will develop your skills in complex analysis and then employ these to find solutions for the electric field and its nature about the triple contact point.

This project is relevant to students with interests in complex analysis and its applications, as well as electrostatics. Background knowledge of complex analysis should be considered a prerequisite. The project will involve some numerics, so some skill in coding is preferred.

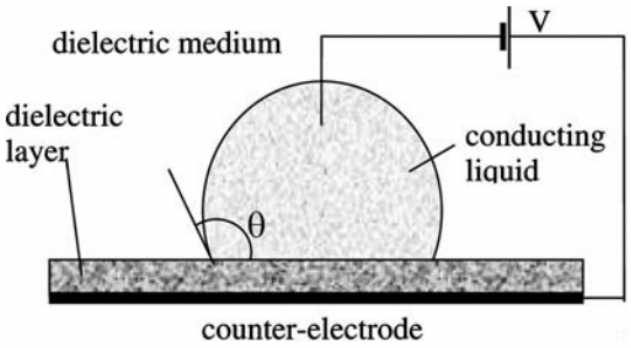


Figure 1: The electrowetting setup with the contact angle θ marked. The triple contact point is the point at which θ is measured about. Figure taken from [2].

References

[1] Chen, L. and Bonaccurso, E., 2014. Electrowetting—From statics to dynamics. Advances in colloid and interface science, 210, pp.2-12.

[2] Adamiak, K., 2006. Capillary and electrostatic limitations to the contact angle in electrowetting-on-dielectric. Microfluidics and Nanofluidics, 2(6), pp.471-480.

Complex variable methods for low-Reynolds number swimming near walls

Dr Sam Brzezicki

This project uses complex variable methods for studying 2D microswimming in Stokes flow (low-Reynolds number flow). The project will begin with learning the complex variable formulation of Stokes flow and then a study of point singularities by a wall (a flat boundary) in the fluid will be conducted. Once a firm understanding of the introductory material has been developed the Crowdy-Or [1] point swimmer model will be introduced and its behaviour in simple geometries will be investigated.

Adjusting this point swimmer so that it includes a selection of different singularities to the Crowdy-Or model and an investigation into how these new singularities behave when in the vicinity of boundaries of the fluid is of interest, as well as extending the portfolio of geometries these swimmer models have been investigated in.

This project is relevant to students with interests in fluid mechanics and complex analysis. Background knowledge of both of these topics should be considered a prerequisite. The project will involve some numerics, so a good command of Python/Matlab is preferred.

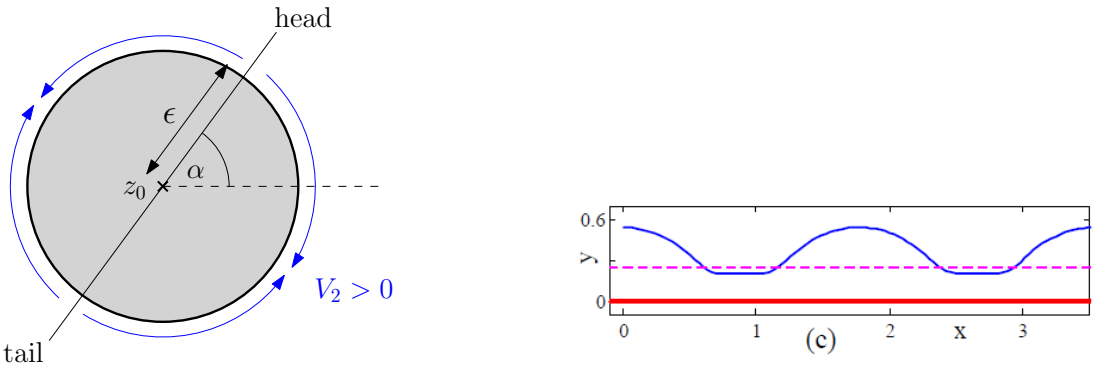


Figure 1: The Crowdy-Or point singularity swimmer (left) with one of its wall bouncing trajectories (right)

References

[1] Crowdy, D.G., Or, Y. 2010 Two-dimensional point singularity model of a low-Reynolds-number swimmer near a wall. *Phys. Rev. E.* 81, 036313.

[2] Obuse, K., Thiffeault, J-L. 2012 A low-Reynolds-number treadmilling swimmer near a semiinfinite wall. In *Natural locomotion in fluids and on surfaces: swimming, flying, and sliding (The IMA Volumes in Mathematics and its Applications)*,155, pp. 197–206. Berlin, Germany: Springer.

Projects with Professor Colin Cotter

Title: Implicit time integration for compatible finite element discretisation of the rotating shallow water equations on the sphere

Description: Compatible finite element methods are a type of discretisation that are tailored towards the requirements of global atmosphere models (and ocean models). They form the foundation of the next generation LFRic weather model at the Met Office, which will become operational for weather and climate simulation there in the next few years. In this project we will investigate a time stepper called TR-BDF2 when applied to these discretisations (used in the context of the rotating shallow water equations which are a 2D model that is often used as a stepping stone towards 3D models). We will make numerical investigations some or all of:
1) the long time properties of the method,
2) the implementation and properties of the "Rosenbrock" version of the method, which requires less linear solves per timestep,
3) high performance solution strategies for the resulting linear and nonlinear algebraic systems.

The project will involve implementing the method using the Firedrake code generation library in Python (www.firedrake.org), and making computational experiments to explore some or all of 1-3. It is not necessary to have previous experience or knowledge of finite element methods, but an enthusiasm for code implementation and creative numerical experiments is important! Firedrake is useful for this type of project since it automates much of the low level implementation aspects and we can concentrate on the interesting parts of the method and algorithm. It can be used on Linux, Mac, or on Windows via Windows Subsystem for Linux.

References:
Gibson, Thomas H., Andrew TT McRae, Colin J. Cotter, Lawrence Mitchell, and David A. Ham. Compatible Finite Element Methods for Geophysical Flows: Automation and Implementation Using Firedrake. Springer Nature, 2019.
Bonaventura, Luca, and A. Della Rocca. "Unconditionally strong stability preserving extensions of the TR-BDF2 method." Journal of Scientific Computing 70, no. 2 (2017): 859-895.

Title: Finite element discretisation of the r-Camassa-Holm equation

Description: The r-Camassa-Holm equation is a 1 (space) + 1 (time) nonlinear partial differential equation, recently introduced by Colin Cotter and Darryl Holm. It has some interesting properties:
1. It has a conserved energy given by the integral of u^r + u_x^r, which is the W^1_r norm (to the power r).
2. It has "singular solutions" with "peaks" corresponding to a jump in the derivative.
When r=2, this equation is called the Camassa-Holm, which is known to form singular solutions in finite time, after which the peaks continue to evolve and interact.
The discretisation of this equation is totally unexplored. This project will investigate some fundamental questions: what is the best form of the equations to discretise? what kind of numerical dissipation is necessary for stable integrations? Do singular solutions emerge in the r>2 case? How can we efficiently solve these equations?

The project will involve implementing the method using the Firedrake code generation library in Python (www.firedrake.org), and making computational experiments to explore some or all of 1-3. It is not necessary to have previous experience or knowledge of finite element methods, but an enthusiasm for code implementation and creative numerical experiments is important! Firedrake is useful for this type of project since it automates much of the low level implementation aspects and we can concentrate on the interesting parts of the method and algorithm. It can be used on Linux,

Mac, or on Windows via Windows Subsystem for Linux. For students who are more interested in analysis, there may also be a possibility to develop some rigorous analysis of the method

Projects with Professor Pierre M Germain

Subject 1: the kinetic wave equation.

The kinetic wave equation describes the dynamics of nonlinear dispersive equations in the regime known as wave turbulence. It is a kinetic equation, which describes how the energy is distributed in phase space, and how the distribution evolves. It is of great physical relevance, since it has been applied to many systems, from plasma physics to nonlinear optics, or waves on the ocean. It is also of great interest for mathematicians, since it provides an entry point into the mysterious world of turbulence.
The aim of this project will be to understand the dynamics of a specific one-dimensional kinetic wave equation, in the space inhomogeneous regime. Local well-posedness will be the starting point, and large-time behavior (scattering?) the aim.

Subject 2: mathematical analysis of thin film equations

The physics of thin films is extraordinarily rich, with a great wealth of phenomena and possible regimes. In many interesting cases, nonlinear dispersive equations can be derived, which have fascinating mathematical properties (solitons, scattering, complete integrability).
The aim of this project will be to carry out a mathematical analysis of some of the models which have been proposed recently, in particular in the work of Papageorgiou. This will include local well-posedness, existence of solitons, variational structure, and possibly large time behavior and the stability of solitons.

Quantum classical correspondence in phase space for systems with non-Hermitian Hamiltonians

Supervisors: Dr Eva-Maria Graefe, Dr Joseph Hall

Suitable for 1 student.

Description

The connection between quantum and classical descriptions of physical systems has been investigated since the advent of quantum mechanics at the beginning of the last century. While much has been learned in over a century, there are still many open questions. It is convenient to compare quantum and classical mechanics in phase space. Phase-space distributions of quantum eigenstates often show close similarities to classical phase-space structures. In this project we are interested in non-Hermitian quantum Hamiltonians, describing systems with loss and gain, for which the quantum-classical correspondence is only beginning to be investigated. The surprising properties of quantum systems with gain and loss (non-Hermitian systems) have sparked much interest recently, and new experimental areas (involving for example optical wave guides, cold atoms, and meta materials) are rapidly emerging.

Plan

We will consider some simple example systems, both chaotic and regular and study the behaviour of the Husimi functions of eigenvectors and other characteristic states of the quantum system, in comparison to classical phase-space structures. We shall also consider the generalisation of phase-space entropies to non-Hermitian systems.

Prerequisites: While this project does not require a big amount of background knowledge, a working knowledge of quantum mechanics and a willingness to use numerical tools (specifically matlab) are prerequisites.

References

(1) B. Mirbach and H. J. Korsch, *Phase Space Entropy and Global Phase Space Structures of (Chaotic) Quantum*, Phys. Rev. Lett. **75** (1995) 362

(2) Steve Mudute-Ndumbe and Eva-Maria Graefe, *A non-Hermitian PT-symmetric kicked top*, New J. Phys. **22** (2020) 103011

Quantum chaos on teardrops - kicked atom molecule conversion

Supervisor: Eva-Maria Graefe

Suitable for 1 student.

Description

The mathematical description of interacting quantum atoms and molecules, which can be converted into one another, and possible dynamical schemes for an effective conversion, is challenging and interesting at the same time. Here we will consider a simple model system with just one quantum state for atoms and molecules, respectively, which leads to a classical phase space that has the shape of a teardrop. The quantum-classical correspondence of this system has been investigated and understood to a fair degree. We will now introduce a further element into the system, by varying some of the parameters periodically in time. In the classical system this can lead to the onset of chaos, and it will be interesting to investigate the fingerprints of this in the quantum description.

Plan

In this project you will familiarise yourself with the description of interacting atoms and molecules in the ground state of an external potential, leading to classical dynamics on unusual phase spaces. You will analyse the resulting dynamics in detail, and then investigate a time-dependent system, using both numerical and analytical tools. Specifically, a quantum phase-space distribution (Husimi distribution) in the sphere will play an important role.

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

References

(1) E. M. Graefe, M. Graney, and A. Rush, *Semiclassical quantization for a bosonic atom-molecule conversion system*, Phys. Rev. A **92** (2015) 012121

(2) F. Haake, M. Kug, and R. Scharf, *Classical and Quantum Chaos for a Kicked Top*, Z. Phys. B **65** (1987) 381

Automating numerical simulation in Firedrake

Supervisor: David Ham

Suitable for one or more students.

Description

The numerical solution of partial differential equations underpins much of computational science and engineering. From weather forecasting to industrial design and from seismology to microfluids, the numerical solution of PDEs is everywhere. Creating numerical simulations requires the combination of advanced techniques from numerical analysis, linear algebra, mathematical optimisation as well as computer science in the form of parallel programming and software optimisation. This has traditionally made the creation of new simulations an exceptionally complex and labour-intensive process. The Firedrake project is a part of a new wave of software tools which take a radically different approach. Instead of relying on mathematicians and engineers to implement new simulations in code, Firedrake takes a mathematical specification of a simulation and uses innovative computer programmes to automatically generate the computer code implementing the model.

By freeing the user from the task of implementing the model, Firedrake makes the creation of more sophisticated simulations achievable. By automating code generation, we can also enable optimisations which would be too labour-intensive or error-prone for many users to attempt themselves. Firedrake is in use by mathematicians, scientists and engineers around the world to simulate a huge range of natural and man-made phenomena. Of course Firedrake can't do everything and there is always user demand for more features and better performance. This generates boundless opportunities for computational maths research projects which, if done well, have global impact on simulation science.

Current opportunities include, but are not limited to:

GPU offload of solvers: Many modern supercomputers rely on graphical processing units (GPUs) for a large proportion of their floating point capability. The PETSc solver library that Firedrake employs has support for executing these solvers on GPUs by first building the matrix on the main CPU and then copying it across to the GPU. In this project you will expose this functionality at the Firedrake level, and construct and apply mathematical performance models to evaluate the resulting performance. This project would suit a student with a strong interest in high performance computing.

Improved automated adjoints: Solving PDEs can be used to simulate real physical systems, but scientists and engineers usually want more than that: they want to evaluate the sensitivities of a system, choose the optimal design or otherwise generate understanding of the system being simulated. What all of these have in common is that they depend on evaluating not just the PDE but the derivative of the PDE with respect to some parameters. This amounts to differentiating the PDE solver and, evaluating it backwards. This is analogous to back propagating a neural net. Firedrake has an automated capability to evaluate adjoint models, but the performance is not optimal in comparison with the forward model. In this project we will understand the adjoint simulation process and evaluate the adjoint against its theoretical performance in order to isolate and improve this situtation. This project would suit a student with an interest in inverse problems and algorithms.

Both of these projects offer the opportunity to develop both mathematical and computational skills in the context of a professional computational mathematics community, and to make contributions that go into production use.

Plan

In each case we will start by learning how to solve the relevant class of problem in Firedrake to the limit of Firedrake's current capabilities. We will then formulate the problems that we would like to be able to solve as a sequence of challenges of increasing complexity to work through. This will provide a graded pathway which enables us to ensure that worthwhile achievements are achieved while allowing space for the student to go further and really excel.

Prerequisites: Interest in PDEs and computational mathematics. You will have taken Finite Elements or plan to take it in the coming year.

References

(1) The Firedrake website `https://firedrakeproject.org`
(2) The Dolfin-adjoint website `https://www.dolfin-adjoint.org/en/latest/`
(3) The PETSc documentation `https://petsc.org/release/overview/`

Time-optimal control of agent-based dynamics

Supervisors: Dante Kalise and Grigorios A. Pavliotis

Description

In this project we will study the synthesis of control laws for agent-based models arising in large animal populations (bird flocks, fish shoal, and sheep) and swarm robotics. The objective is to determine optimal control signals which are able to steer the population towards a desired state, e.g. a certain spatial configuration or flocking state. For this, we will follow a dynamic optimization approach, deriving optimality conditions which characterize an optimal intervention. In particular, we will focus on the synthesis of optimal controls which are able to achieve the objective in a minimum amount of time. The derivation of optimality conditions guides the construction of numerical methods for an effective control synthesis. Moreover, we will explore the control synthesis as the number of agents grows, paving the way for a mean-field modelling of the time-optimal control problem.

A background on dynamical systems, numerical analysis, and optimisation/control is desirable.

Plan

The project is split into three stages:

(1) Mathematical modelling of collective behaviour phenomena: animal behaviour, agent-based models, and swarm robotics.
(2) Time-optimal control, optimality conditions for agent-based dynamics.
(3) Computational synthesis of control laws through dynamic optimization. Mean-field scaling of the control problem.

References

(1) Y. Chen and T. Kolokolnikov. *A minimal model of predator-swarm interactions,* J. R. Soc. Interface 11(94):20131208 (2014).
(2) D. Strömbom, R.P. Mann, A.M. Wilson, S. Hailes, J. Morton, D.J. Sumpter, and A. J. King. *Solving the shepherding problem: heuristics for herding autonomous, interacting agents,* J. R. Soc. Interface 11(100):20140719 (2014).
(3) M. Bongini, M. Fornasier, M. Hansen, and M. Maggioni . *Inferring interaction rules from observations of evolutive systems I: The variational approach,* Math. Models Methods Appl. Sci. 27(5):909–951 (2017).
(4) R. Bailo, M. Bongini, J.A. Carrillo and D. Kalise. *Optimal consensus control of the Cucker-Smale model,* IFAC-PapersOnLine 51(13)(2018):1–6.

Optimal vibration control of slender structures

Supervisor: Dante Kalise

Description

In this project we will study active vibration control strategies for slender structures such as bridges, trusses, and aircraft wings. We will study this problem in the framework of PDE-constrained optimization, where the control is designed by optimizing a performance index (vibration mitigation plus control effort) constrained to a PDE governing the structural vibration dynamics. Since standard structural vibration models are linear, after a suitable discretization the active vibration control problem can be cast as a Linear-quadratic Regulator (LQR) problem, and can be solved trough a large-scale Algebraic Riccati Equation. As an extension, we will study a mathematical formulation for the optimal location and design of sensors and actuators in the framework of bi-level optimization.

Plan

The project is split into three stages:

(1) Modelling and approximation of structural vibration phenomena: beam and plate models, time/frequency-dependent formulations, FEM and spectral approximation.
(2) PDE-constrained optimization. The LQR problem for structural dynamics, optimality conditions for the stationary problem. Numerical approximation of large-scale control problems.
(3) Actuator/sensor aspects: piezoelectric actuators, optimal actuator/sensor location and design.

A background/interest on computational mathematics and mathematical modelling with PDEs is essential.

References

(1) E. Hernández, D. Kalise and E. Otárola. *Numerical approximation of the LQR problem in a strongly damped wave equation,* Computational Optimization and Applications, 47:161–178 (2010).
(2) E. Hernández, D. Kalise and E. Otárola. *A locking-free scheme for the LQR control of a Timoshenko beam,* J. Comput. Appl. Math. 235(5): 1383-1393 (2011).
(3) M. S. Edalatzadeh, D. Kalise, K. A. Morris and K. Sturm. *Optimal Actuator Design for the Euler-Bernoulli Vibration Model Based on LQR Performance and Shape Calculus,* IEEE Control. Syst. Lett. 6: 1334-1339 (2022).

Deep Neural Networks for Real-time Trajectory Planning

Supervisor: Dante Kalise

Description

Different problems in robotic locomotion can be studied in the framework of optimal control theory. For example, we can look for a set of actions (controls) which take a drone from point A to B by minimizing the amount of time or energy that is required to complete the task. These control signals are often expressed as feedback laws, that is, real-time actions which can be implemented solely based on the current state (position, velocity) of the robot. In this project, we will develop a deep learning formulation of the optimal trajectory planning problem outlined above. y combining methods from dynamical systems, control theory, and polynomial systems, we will generate a synthetic dataset of optimal input-output pairs. This synthetic dataset will be used to cast a supervised learning problem to approximate an optimal feedback law to be applied in real time after a measurement of the current state of the system.

Plan

The project is split into three stages:

(1) A brief introduction to optimal control: minimum time formulation, bang-bang controls, switching structures.
(2) Parametrizing optimal control problems as nonlinear and/or polynomial systems. Solution strategies via iterative methods or computer algebra.
(3) Synthetic data generation and supervised learning approaches for synthesizing feedback laws. Applications in robotic locomotion.

Prerequisites: basic knowledge of dynamical systems, computational simulation tools, and machine learning (DNNs, supervised learning). Programming skills in Matlab and/or Python. Willingness to learn about polynomial systems and/or computer algebra is desirable.

References

(1) U. Walther, T. T. Georgiou and A. Tannenbaum. *On the computation of switching surfaces in optimal control: a Grobner basis approach,* in IEEE Transactions on Automatic Control, vol. 46, no. 4, pp. 534-540, April 2001, doi: 10.1109/9.917655.
(2) B. Karg and S. Lucia. *Efficient Representation and Approximation of Model Predictive Control Laws via Deep Learning*, in IEEE Transactions on Cybernetics, vol. 50, no. 9, pp. 3866–3878, Sept. 2020, doi: 10.1109/TCYB.2020.2999556.
(3) B. Azmi, D. Kalise and K. Kunisch. *Optimal Feedback Law Recovery by Gradient-Augmented Sparse Polynomial Regression,* in Journal of Machine Learning Research, 22(48):1–32, 2021.

Projects with Dr Omer Karin

Project: theory of self-organized memory

Background. A remarkable property of biological systems is their ability to record and maintain long-term memories, as in the immune system, the brain, and epigenetic memory. An outstanding question is how long-term memory comes about in living systems from their underlying (biochemical) interactions.

We recently addressed this by studying long-term memory in a unique model system: the transfer of information across generations in worms (a.k.a transgenerational epigenetic inheritance). We showed that long-term memory in this system comes from the coupling by competition of many simple dynamical systems which act as “memory units". The system self-tunes to the vicinity of a transition to bistability, where it has unique properties that are both functionally important and capture distinct experimental phenomenology. As the assumptions underlying this self-organized memory model are quite general in biological contexts, we expect it to be relevant to other systems as well (including immune memory).

Project description. The goal of this project is to improve our theoretical understanding of the self-organized memory phenomena, with an emphasis on understanding the consequences of the biologically-relevant heterogeneity between memory units (e.g. cells or genes). Examples of questions include- how does heterogeneity affect the composition of the memory pool over time? How can we detect heterogeneity in datasets? What are the implications of different forms of heterogeneity (e.g. heterogeneity in internal parameters or in coupling)? How can heterogeneity be exploited by the memory system (e.g. by selectively retaining relevant memories) and how can it be attacked by parasitic elements?

The project will involve both analytical and numerical components, as well as the possibility of using insights to analyze experimental data.

Prerequisites. Familiarity with methods from nonlinear dynamics and stochastic processes is desirable, as well as the ability to code numerical simulations (e.g. in python or matlab). A background in biology is not necessary.

Project: reinforcement learning in moving animals

Background. Mathematical theory has traditionally played an important role in understanding the behavior of moving organisms.

Simple organisms (e.g. bacteria) navigate according to the sensing of an input field which consists of diffusible signal molecules, signifying for example the locations of food sources or toxins. An outstanding conclusion is that different organisms often share a similar navigational strategy- they navigate by adjusting their movement statistics according to the temporal logarithmic derivative of the input field, resulting in accumulation around peaks of “attractant” molecules and away from “repellant” molecules.

In more complex organisms, including mammals, an important regulator of behavior is dopamine transmission in the brain. Here an influential theoretical framework has been reinforcement learning, which describes how optimal choice behavior can be achieved by an agent who is learning about the consequences of actions through rewards and punishments. The deep link between reinforcement learning algorithms (based on ideas from optimal control / dynamic programming) and learning is motivated by the remarkable correspondence revealed in experiments between dopamine, and the reward prediction error signal in reinforcement learning algorithms.

We recently showed that in fact, both frameworks are relevant for understanding the dopamine system (and therefore learning and behavior of animals). While the reinforcement learning framework captures important aspects of the dopamine system, many other puzzling observations (in mice, primates, and humans) are in fact much more consistent with our knowledge of navigation in simple organisms - specifically, dopamine appears to modulate

movement statistics in response to the temporal logarithmic derivative of an input field corresponding to expectations about rewards.

Project description. While both frameworks are relevant for the dopamine system, they are apparently incompatible - for start, reinforcement learning algorithms focus on discrete decisions and do not take into account the movement of the organism. The goal of this project would be to ask whether our knowledge of (continuous) stochastic navigation can be synthesized with reinforcement learning.
For this, the project will focus on developing and testing algorithms that synthesize our knowledge of the dopamine system, and evaluating their performance in relation to “classical” reinforcement learning algorithms, as well as possibly experiments on animal behavior.

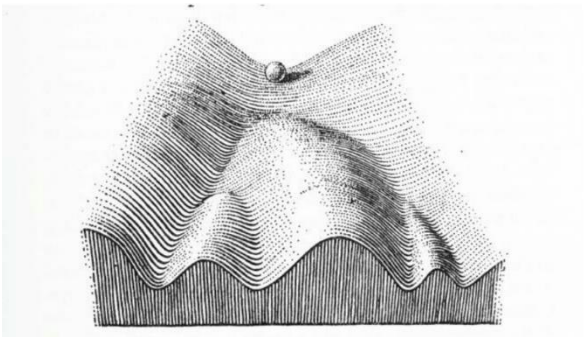
Prerequisites. Solid programming skills are essential; familiarity with ideas from reinforcement learning, control theory, and signal processing will be beneficial.

Project: reversible transitions in stem cell dynamics

Background. The cells in our body our produced from a single fertilized egg through processes of replication and differentiation. Similarly, the many cells in our body (like our immune cells or skin cells) are constantly turned over and re-made from the replication and differentiation of dedicated stem cells. An attractive metaphor for this process has been the *Waddington Landscape*, which compares the differentiation of a stem cell to a marble ball rolling down the slope of a hill and entering valleys, corresponding to the commitment to differentiated cell types.
While this picture is intuitive and appealing, our actual knowledge of the behavior of stem cells deviates substantially from this picture. For one, stem cells tend to transition reversibly between states with a different propensity for differentiation. This process remains poorly understood, especially with respect to the dynamic behavior of the transitions and their functional importance.

Project description. The goal of this project will be to use measurements on single cells, such as single-cell transcriptomics, to characterize reversible transitions in stem cells. The project will include both the analysis of large biological datasets (including the application of cutting-edge computational methods, and the development of ad-hoc relevant computational methods) and dynamical modeling.

Prerequisites. Familiarity with python / R for data analysis, as well as familiarity with nonlinear dynamics, and interest in data-driven modeling.



Title: Dynamics of passive and active filaments in viscous fluids
Supervisor: Dr Eric E Keaveny
Description: Filaments are slender, flexible objects that deform by bending and twisting and whose shape is provided by a one-dimensional curve. Collections of microscopic filaments immersed in a viscous fluid are often encountered in biological settings, as they are often used in the cellular propulsion, as well as in engineering applications where they are a key ingredient in polymeric fluids.
The project involves simulating the dynamics of filaments as they move and interact through a surrounding viscous fluid. The students will utilise methods and codes (written in MATLAB) developed for this task. The project can be tailored to the students interests, but possible directions include:

1. Filament bundling
2. The syncronised movement of active filaments
3. Tumbling and dynamics of sedimenting filaments
4. The motion of filaments in external flows.
5. Filament dynamics in external fields.
6.

The first part of the project will be to familiarise yourself with the code and understand the computations that it performs. This will involve studying our paper which outlines the methodology and reproducing some of the results within it. The second part will entail modifying and testing the code to generate results related to one of the directions listed above. Once this is done, results can be generated and written up.
Reference: Simon F. Schoeller, Adam K. Townsend, Timothy A. Westwood, Eric E. Keaveny, Methods for suspensions of passive and active filaments, Journal of Computational Physics, Volume 424, 2021,109846.
Codes: https://github.com/ekeaveny/filaments

> ekeaveny/filaments: Codes associated with 'Methods for suspensions of passive and active filaments' - GitHub
> filaments: README. Supplementary Matlab/Octave code to 'Methods for suspensions of passive and active filaments', 2019, by SF Schoeller, AK Townsend, TA Westwood & EE Keaveny.. 1. Whom do I talk to? The authors can be contacted at: Simon Schoeller: simon.schoeller14@imperial.ac.uk Adam Townsend: adam.townsend@imperial.ac.uk Tim Westwood: t.westwood16@imperial.ac.uk
> github.com

Title: Dynamic mode decomposition of complex fluid flows
Supervisor: Dr Eric E Keaveny
Description: Complex fluids are fluids that contain suspended microscopic particles, such as polymer molecules, that give the fluid a nonlinear mechanical response to applied forces. As a result, even in the absence of inertia, these fluids can exhibit intricate and complicated turbulence-like flow patterns when subjected to an external force.
The project involves using the data-driven technique \textit{dynamic mode decompostion} (DMD) to characterise these flow patterns. The data used in the project will be obtained from complex fluid simulations related to:

1. viscoelastic instabilities exhibited by polymeric fluids, or

2. instabilities found for suspensions of swimming bacteria.
3.

The first part of the project will be to familiarise yourself with DMD and understand the computations that it performs. This will involve studying the book listed in the references which outlines the methodology, and reproducing some of the results within it. The second part will entail adapting and using the codes presented in the book to analyse the data sets related to the one of the simulations listed above. Once this is done, results can be generated and written up.

References: Kutz, J. N., Brunton, S. L., Brunton, B. W., & Proctor, J. L. (2016). Dynamic mode decomposition: data-driven modeling of complex systems. Society for Industrial and Applied Mathematics.

Projects in Industrial mathematics: Dr. Toby Kirk

1. *Nonstationary impedance spectroscopy for parameter determination in Li-ion battery models*

The mathematical modelling of lithium-ion batteries is becoming increasingly important in recent years, in order to understand how they work, how to improve them, and how they degrade/fail. Electrochemical models [1] are physically realistic, but their parameters are difficult and time consuming to determine. Impedance spectroscopy (periodic alternating current (AC) inputs), at a fixed state of charge, is the prevailing technique to determine and understand kinetic or reaction parameters (short time scales) [2]. But pulse current discharge (DC) and relaxation is a better technique to determine Li diffusivities and electrode particle-size distributions (long time scales). This project will explore the use of impedance and discharge/relaxation techniques simultaneously, aiming to combine the best of both in a single experiment. We will use the asymptotic method of multiple timescales applied to an electrochemical model [3]. We will verify when this timescale separation is valid by comparing to brute force time-dependent computations, and investigate the advantages to parameter estimation.

Prerequisites: numerical solution of PDEs, asymptotic methods, Matlab or Python. Knowledge of reaction-diffusion equations, FFTs, parameter estimation methods is useful but not necessary.

[1] G. Plett, Battery Management Systems: Volume I Battery Modeling, *Artech House*, 2015
[2] Barsoukov & Macdonald, Impedance Spectroscopy: Theory, Experiment, and Applications, 2nd edn, *Wiley*, 2005
[3] Kirk, Evans, Please & Chapman, *SIAM Journal on Applied Mathematics*, 82(2), 2022, online

2. *Asymptotic reduced models for convection in longitudinal-fin heat sinks*

Heat sinks are ubiquitous in electronic devices and are used to spread heat away from strong localised heat sources, such as CPUs. The most common form of heat sink consists of an array of thin metal fins. In conjunction with fans, which blow air between the fins, heat is removed by conduction and convection. Modelling usually involves the solution of 2D (or 3D) partial differential equations for the flow and temperature fields, and is purely numerical giving limited physical insight [1]. But the fins are typically tall and closely packed—a property never before exploited. We will explore this “closely packed” limit using asymptotic methods, to derive reduced-order approximations to the flow and temperature fields, where the temperature may show fast variation between the fins, but slow variation along the fins. We will compare the asymptotic solutions to the full 2D solution, computed using spectral (e.g. Chebyshev collocation) or finite element methods. The project could also be extended to the 3D developing problem, close to the heat sink inlet [2]. The project will involve a mixture of analytical and numerical work (and may have the opportunity to collaborate with mechanical engineers).

Prerequisites: numerical solution of PDEs, asymptotic methods, Matlab or Python.

[1] G. Karamanis & M. Hodes, *Journal of Thermal Science and Engineering Applications*, 8(4):041011, 2016
[2] G. Karamanis & M. Hodes, *Journal of Heat Transfer*, 141(8), 2019.

Section: Applied.

Random Dynamical Systems

Supervisor: Jeroen Lamb (jswlamb@imperial.ac.uk)

Suitable for various students.

Description

These projects engage with the research of PhD students Matheus Manzatto, Giuseppe Tenaglia, Hugo Chu, Nero Li and/or Bernat Bassols Cornudella. Dr Martin Rasmussen and/or Prof Dmitry Turaev may co-supervise.

Random dynamical systems are dynamical systems driven by a noise. For instance, the following questions may be pursued:

- Conditioned dynamics: one may study random dynamical systems constrained by the condition that orbits do not leave some bounded subset of the state space. Conditioned versions of Lyapunov exponents, entropy and invariant measures are studied and their implications for dynamical behaviour.
- Learning random dynamics. Can the equations of motion of a random dynamical system be learned from observations of trajectories?
- The route to chaos in random dynamical systems: how do random dynamical systems develop sensitive dependence on initial conditions?
- Topological bifurcations of random dynamical systems with bounded noise: if noise is bounded, random dynamical systems may display bounded localized attractors. We study the behaviour such attractors when parameters are varied.

Prerequisites: These projects are in the field of dynamical systems; specific techniques depend on the type of project pursued. It is possible to give the project a more analytical (theoretical) or computational flavour.

Project with Dr Eeltje C Nijiholt

From Networks to Hypernetworks

Networks play a major role throughout science and engineering! Think about the brain, the internet, electronic circuits, ecosystems, social media, and many more examples. From a mathematical point of view, it is no mystery that these structures are so often featured, as they are well-known to support remarkable phenomena. This is especially true for network dynamical systems, where quantities that change over time can display interesting dynamical behavior when coupled together, even though the behavior of the individual units may be completely unremarkable. More mysterious is precisely how network structure causes this behavior to occur.

Recently, another structure has garnered significant attention in the scientific community: that of a *hypernetwork*. Precise definitions vary, but the main theme is that instead of one unit influencing another through a connection, we now allow for multiple nodes to communicate via one *hyperconnection*. This brings new challenges with it. For instance, what is a workable definition of a hypernetwork? Are there dynamical properties of hypernetworks that are not possible for classical networks, or are they just two sides of the same coin?

This project is about hypernetwork dynamical systems, with a focus on dynamically invariant spaces and bifurcations, and the contrast with classical networks in this regard. The student will learn to apply techniques from dynamical systems theory to a set-up that is directly motivated by "real world" systems. Moreover, they will explore a topic that has just recently become very popular in the (network) dynamical systems community.

Project with Dr Eeltje C Nijiholt

Understanding Linear Network Maps through Representation Theory

Networks are all around us! They are used as models for the brain, ecosystems, electronic circuits, gene interactions, coupled lasers, and many more. It is no coincidence that these structures play such an abundant role in nature and engineering, as they are able to support rich mathematical phenomena that are otherwise highly unusual. This is especially true for network dynamical sys-tems, where quantities that change over time can display interesting dynamical behavior when coupled together, even when the behavior of the individual units may be completely unremarkable.

The first step in understanding this –and indeed the starting point of many powerful techniques from dynamical systems theory– is an investigation of *lin-ear* network systems. As expected, network structure will likewise put con-straints on linearized systems, which in turn influence eigenvalue-multiplicity, eigenspaces and so forth. Recent results have shown that a major role is played by representation theory in this regard. In essence, the linear maps of many network systems can be viewed as precisely those that respect the representa-tion of a monoid. This allows us to analyze spectral properties of network maps by relating them to sub-representations of this hidden symmetry.

This project offers a unique blend of dynamical systems theory, algebra and combinatorics, while keeping close to the "real world" of network systems. It does not lean too heavily on any of these aforementioned disciplines and allows the student a great deal of flexibility, by looking for instance into developing a computer program or exploring the geometrical side of these symmetries, if time permits.

Project with Dr Eeltje C Nijiholt

Structure Preserving Reduction Techniques

Bifurcations are sometimes described as the "bread and butter" of the dynamical systems community. They can roughly be described as sudden, qualitative changes in a system when one or more parameters are changed, and they are of enormous importance in many dynamical models. Examples include the climate, opinion dynamics, food-webs, chemical reactions and many more.

A common problem in bifurcation theory –and indeed in the field of dynam-ical systems theory in general– is simply dealing with the size of the system. When there are too many variables present, or when the dynamical equations are too complicated, it can be hard to see how the system behaves or reacts to parameter-changes. For this reason, various *reduction techniques* have been developed. They take a dynamical system and output a smaller or otherwise simpler system with the same dynamical properties under investigation. Of course there are limitations to such techniques. Most notably, if a dynamical system has any kind of additional structure, for instance a symmetry or an un-derlying network form, then we would much like to preserve these features in such reductions. A recent technique allows for just that, by translating many features into geometric properties of the system, using so-called quiver repre-sentations.

This project focusses on the consequences of this new framework, mostly with respect to bifurcations. It involves an interesting mix of dynamical systems theory, geometric and algebraic techniques, without leaning too heavily on any of these. Within this topic, the student is free to explore different directions, such as an application to network dynamical systems or a more in-depth look at the underlying representation theory.

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

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

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:

$$\left(\begin{array}{c|cc|ccc|ccccc}
\times & \times & \times & & & & & & & & \\
\hline
\times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & & & & & \\
\hline
 & \times & \times & \times & \times & & \times & \times & & & \\
 & \times & \times & \times & \times & \times & \times & \times & \times & & \\
 & & \times & & \times & \times & & \times & \times & \times & \\
\hline
 & & & \times & \times & & \times & \times & & & \\
 & & & \times & \times & \times & \times & \times & \times & & \\
 & & & & \times & \times & & \times & \times & \times & \\
 & & & & & \times & & & \times & \times &
\end{array}\right)
\left(\begin{array}{c} u_{00} \\ \hline u_{10} \\ u_{11} \\ \hline u_{20} \\ u_{21} \\ u_{22} \\ \hline u_{30} \\ u_{31} \\ u_{32} \\ u_{33} \end{array}\right)
=
\left(\begin{array}{c} f_{00} \\ \hline f_{10} \\ f_{11} \\ \hline f_{20} \\ f_{21} \\ f_{22} \\ \hline f_{30} \\ f_{31} \\ f_{32} \\ f_{33} \end{array}\right)$$

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 the left of Figure 1 for the Helmholtz equation.

The MSc. project consists of extending this methodology to solve PDEs on three-dimensional simplices, e.g., $S = \{(x, y, z) : 0 \le x, y, z \le 1, 0 \le x + y + z \le 1\}$, 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 using recent generalisations of the recurrence relationships derived for two-dimensional multivariate orthogonal polynomials to three-dimensions, using these to construct matrix representations of the operators, implementing fast linear algebra routines for the resulting sparse matrices, and solving some simple model problems like three-dimensional Poisson equation and Helmholtz equations.

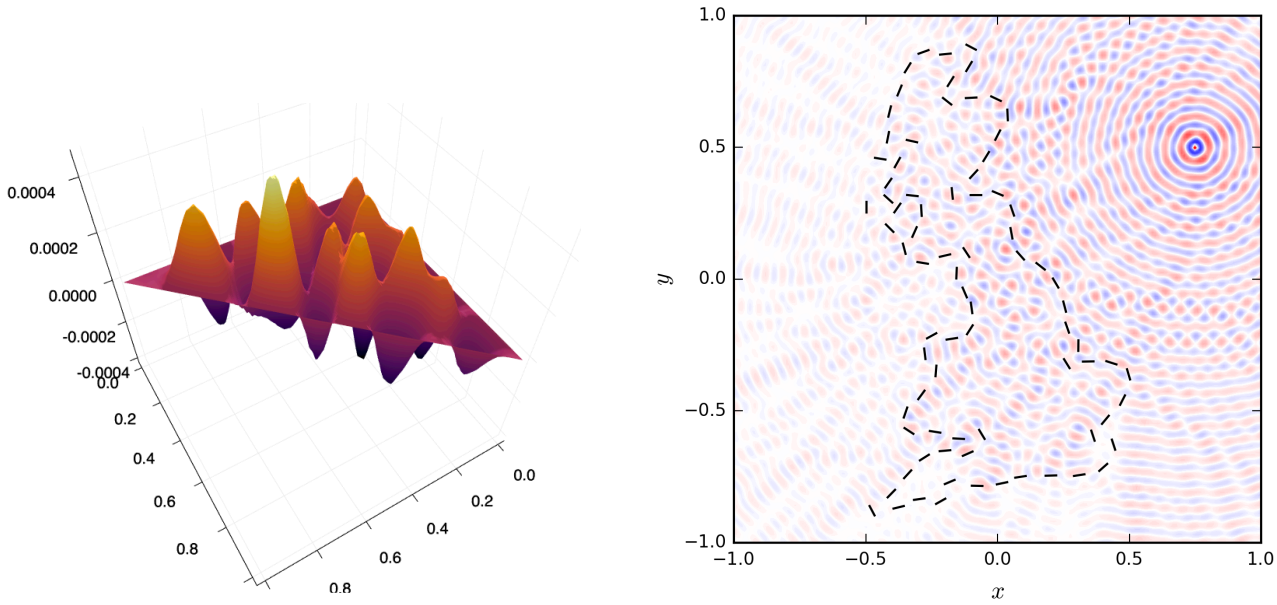


Figure 1: Solution to Helmholtz equation in a triangle (left). Acoustic scattering off Britain (right).

Cauchy transforms on wedges and applications to scattering

Supervisor: Dr Sheehan Olver

This project investigates computation of the Cauchy transform

$$\frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{f(\zeta)}{\zeta - z} \, \mathrm{d}\zeta$$

where $\Gamma = (0,1) \cup (0, c\mathrm{e}^{\mathrm{i}\theta})$ is a *wedge*. In the case of a right-angle ($\theta = \pi/2$) this is possible using a new mapping formula to an easier geometry, embedded in a two-sheeted Riemann surface. The project consists of generalisation to non-right-angles, beginning with rational angles mapping to an multiple-sheeted Riemann surface.

The second aspect is applying such mappings to solving scattering problems, for example acoustic scattering of obstacles, see the right of Figure 1 for an example *without corners*. Green's representation theorem is a way of reducing PDEs to singular integrals involving logarithmic kernels, which is closely linked to the Cauchy transform. By considering carefully the singularities of the solutions we can solve PDEs with very high accuracy. Thus the project will investigate application of the Cauchy transform mappings to the case where the geometries have corners.

PROFESSOR GRIGORIOS A. PAVLIOTIS

Variance reduction methods for Markov Chain Monte Carlo

Markov chain Monte Carlo (MCMC) is one of the most widely used and versatile methods for sampling from probability distributions that are known up to the normalisation constant, in particular in high dimensional spaces. MCMC is based on simulating a Markov chain that is ergodic with respect to the distribution from which we want to sample. The performance of an MCMC algorithm depends on the time it takes for the Markov chain to reach the distribution from which we want to sample and on the asymptotic variance of the chain. For complicated, multimodal distributions in high dimensional spaces, it is quite often the case that the computational cost for obtaining accurate samples using the MCMC methodology is computationally prohibitive. To reduce the computational cost and to improve the performance of the MCMC algorithm, it is necessary to employ bias correction and variance reduction techniques. The goal of this project will be to study, analyse and to implement variance reduction techniques for MCMC algorithms. Applications to Bayesian inference will also be explored.

References

Huang, Lu-Jing; Liao, Yin-Ting; Chen, Ting-Li; Hwang, Chii-Ruey Optimal variance reduction for Markov chain Monte Carlo. SIAM J. Control Optim. 56 (2018), no. 4, 2977–2996.

Mira, Antonietta; Solgi, Reza; Imparato, Daniele Zero variance Markov chain Monte Carlo for Bayesian estimators. Stat. Comput. 23 (2013), no. 5, 653–662.

Papamarkou, Theodore; Mira, Antonietta; Girolami, Mark Zero variance differential geometric Markov chain Monte Carlo algorithms. Bayesian Anal. 9 (2014), no. 1, 97–127.

Rey-Bellet, Luc; Spiliopoulos, Konstantinos Improving the convergence of reversible samplers. J. Stat. Phys. 164 (2016), no. 3, 472–494.

Stochastic Gradient Descent in Continuous Time

The methods and models of machine learning are rapidly becoming de facto tools for the analysis and interpretation of large data sets. The ability to synthesise and simplify high-dimensional data raises the possibility that neural networks may also find applications as efficient representations of known high-dimensional functions. Training a given neural network remains one of the central challenges in applications due to the slow dynamics of training and the complexity of the objective function. Parameter optimisation in machine learning typically relies on the stochastic gradient descent algorithm (SGD), which makes an empirical estimate of the gradient of the objective function over a small number of sample points. In order to study the properties of stochastic gradient descent for neural network optimisation, it is possible to recast the standard training procedure in terms of a system of interacting particles. It is then possible to use tools from stochastic differential equations and statistical mechanics to study the improve methodologies for the training of neural networks. The goal of this project will be to study recent works on the dynamical study of the training of neural networks and to implement some of the proposed methodologies for improving the performance of the SGD algorithm.

Sirignano, Justin; Spiliopoulos, Konstantinos Mean field analysis of neural networks: a central limit theorem. Stochastic Process. Appl. 130 (2020), no. 3, 1820–1852.

Sirignano, Justin; Spiliopoulos, Konstantinos Mean field analysis of neural networks: a law of large numbers. SIAM J. Appl. Math. 80 (2020), no. 2, 725–752.

Parameters as interacting particles: long time convergence and asymptotic error scaling of neural networks
G Rotskoff, E Vanden-Eijnden
Advances in neural information processing systems, 7146-7155 (2018)

Neural networks as interacting particle systems: Asymptotic convexity of the loss landscape and universal scaling of the approximation error
GM Rotskoff, E Vanden-Eijnden stat 1050, 22 (2018)

MSc projects with Gunnar G. Peng and Ory Schnitzer

Useful prerequisites include a background in fluid dynamics and asymptotic methods.

A. Weakly nonlinear dynamics of active particles and drops

A submerged active particle or drop that produces a chemical on its surface can interact with the resulting chemical field to drive flow and motion of the particle/drop. Theoretical models coupling the Stokes flow of the fluid to the advection–diffusion equation of the chemical [1,2] predict that an isotropic particle/drop spontaneously self-propels in an arbitrary direction if the Péclet number (a parameter that measures the relative strengths of advection and diffusion in the system) exceeds the critical value Pe = 4. Recently, we have derived a reduced model for the dynamics of an active particle using a weakly nonlinear expansion of the full equations in the limit $\mathrm{Pe} \to 4$, which allows theoretical analysis and efficient numerical simulation of the dynamics of the particle in various situations [3,4], and we have an in-house Matlab code that can perform these simulations for one or more particles.

This project can be taken in different directions depending on the interests of the student. One possibility is to adapt the model to active drops instead of particles, which are the more experimentally relevant case. This entails modifying our particle-scale expansion to account for the Stokes flow inside the drop, as well as modified boundary conditions on its surface. Further extensions could account for the deformation of the drop surface, and for the drop being a liquid crystal. Alternatively, the model could be modified to account for multiple particles with different properties, which would require modifying the numerical coefficients at various stages in the analysis and in our code. This would allow analysis and simulation of asymmetric droplet collisions, which have previously been studied using full numerical simulations for axisymmetric head-on collisions only [5]. A third possibility is to study the dynamics of a particle confined to a channel or tube, for which limited full numerical results exist [6]. Our numerical code could straightforwardly be modified to handle a rectangular cross-section using the method of images, while a circular cross-section would require more sophisticated analysis.

[1] S. Michelin, E. Lauga and D. Bartolo, Spontaneous autophoretic motion of isotropic particles, Phys. Fluids, 25(6), 061701, 2013

[2] S. Michelin, Self-Propulsion of Chemically Active Droplets. Annu. Rev. Fluid Mech., 55, 2022

[3] O. Schnitzer, Weakly nonlinear dynamics of a chemically active particle near the threshold for spontaneous motion. I. Adjoint method, arXiv:2205.06136, 2022

[4] G. G. Peng and O. Schnitzer, Weakly nonlinear dynamics of a chemically active particle near the threshold for spontaneous motion. II. History-dependent motion, arXiv:2211.09467, 2022

[5] K. Lippera, M. Benzaquen, S. Michelin, Bouncing, chasing, or pausing: Asymmetric collisions of active droplets, Phys. Rev. Fluids, 5(3), 032201, 2020

[6] F. Picella and S. Michelin, Confined self-propulsion of an isotropic active colloid, J. Fluid Mech., 933, 2022

B. Stability of an electrified fluid interface

This project is motivated by fundamental open problems in the theory of electrohydrodynamic drop deformation in an external electric field. The scenario of interest is that where the interior and exterior fluids are both weakly conducting liquids (e.g., oils), which are well described by the "leaky-dielectric" model of G. I. Taylor and J. R. Melcher [1]. The case of a weak field has been well understood since the 1960s following seminal work by G. I. Taylor [2]. In contrast, the various instabilities and nonlinear dynamical phenomena experimentally observed under strong applied fields remain poorly understood (see the review article [3] and references therein). In particular, under certain conditions on the material properties, and past a critical electric-field magnitude, the drop is observed to spontaneously rotate. For high viscosity drops, this spontaneous rotation agrees with the theory of "Quincke rotation" developed for solid particles [4]. In contrast, there is no theory describing the Quincke rotation of low viscosity drops. Simulations suggest the formation of intense surface-charge gradients at the equator and the possibility of shock-type singularities, while experiments in this case show that the onset of rotation is preceded by a short-wave instability leading to the formation of an equatorial belt of rotational convection cells.

The goal of this project is to gain preliminary insight into the above problems by studying the stability and nonlinear dynamics of a nominally flat electrified interface between two leaky dielectric fluids in the presence of an applied tangential electric field and a stagnation flow, a scenario which naively mimics the near-equatorial conditions in the drop problem. Our motivation is similar to that in [5], however we shall initially consider a simplified formulation neglecting deformation of the interface. Thus, the governing equations are the Stokes and Laplace equations for the fluid flow and electric potentials in each phase, along with nonlinear conditions at the interface including a surface-charge conservation equation and a tangential-stress balance. In contrast to [5], we will aim to go beyond a linear stability analysis to study the weakly nonlinear formation of convections cells near the onset of instability as well as the strongly nonlinear formation of surface-charge shock layers.

[1] J. R. Melcher and G. I. Taylor, Electrohydrodynamics — a review of the role of interfacial shear stress, Annu. Rev. Fluid Mech., 1, 111–146, 1969

[2] G. I. Taylor, Studies in electrohydrodynamics. I. Circulation produced in a drop by an electric field, Proc. Royal Soc. A, 291, 159–166, 1966

[3] P. Vlahovska, Electrohydrodynamics of drops and vesicles, Annu. Rev. Fluid Mech., 51, 1, 2019

[4] T. B. Jones, Quincke rotation of spheres, IEEE trans. ind. app., 4, 845-849, 1984

[5] M. Firouznia et al., Instability of a planar fluid interface under a tangential electric field in a stagnation point flow, J. Fluid Mech., 931, A25, 2022

MSc Projects 2022/23

Dr Martin Rasmussen (m.rasmussen@imperial.ac.uk)

Project 1. Resilience in dynamical systems. Resilience describes how much a dynamical system is away from a bifurcation point where the behaviour of the system changes fundamentally. Several concepts of resilience have been described in the literature. This project builds upon the recently developed notion of intensity, which has been explored for continuous time in [1] and for discrete time in [2]. The approach studies pertubations of the dynamics using a set-valued or control system. Intensity has the advantage that it is a purely dynamical quantity and for this reason more meaningful than other approaches. This project aims first at understanding how the continuous-time theory is related to the discrete-time approach. This is of particular importance when one uses discretisations. Moreover, the project aims at extending the theory from determistic dynamical systems to random dynamical systems. While for random systems with bounded noise, such an extension seems straightforward (at least conceptually), it needs to be explored how these ideas extend to systems with unbounded noise and also to certain questions for bounded noise systems.

[1] K.J. Meyer and R.P. McGehee, *Intensity – a metric approach to quantifying attractor robustness in ODEs*, 2020, `https://arxiv.org/pdf/2012.10786.pdf`.

[2] R.P. McGehee, *Some metric properties of attractors with applications to computer simulations of dynamical systems*, 1988, `http://www-users.math.umn.edu/~mcgehee/publications/McGehee1988p/index.html`.

Project 2. Rate-induced tipping in discrete-time dynamical systems. Tipping points describe bifurcations where the output of a dynamical system changes disproportionately compared to the change in the parameter. In [1], several mathematical mechanisms for tipping have been proposed, including rate-induced tipping, where a system is pushed across a bifurcation point through a nonautonomous change in the parameter that is nonadiabatic, i.e. fast enough, so that it cannot be regarded as a constant parameter in the dynamics. This project aims at understanding rate-induced tipping in the discrete-time context and builds on the results obtained by

PhD student Michael Hartl [2]. In contrast to the continuous-time case, the discrete-time case is almost unexplored and more interesting, since one can observed non-intuitive behaviour already in one dimension.

[1] P. Ashwin, S. Wieczorek, R. Vitolo, and P. Cox, *Tipping points in open systems: bifurcation, noise-induced and rate-dependent examples in the climate system*, Philosophical Transactions of the Royal Society A – Mathematical, Physical, and Engineering Sciences **370**(1962), 2012.

[2] M. Hartl, *Non-autonomous Random Dynamical Systems: Stochastic Approximation and Rate-Induced Tipping*, 2019, `https://spiral.imperial.ac.uk/bitstream/10044/1/73914/1/Hartl-M-2019-PhD-Thesis.pdf`.

Waves and turbulence 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. These flows can exhibit a range of complex phenomena, and the aim of this project is to use simulations of pedestrian flows to investigate these dynamics. You will simulate pedestrian flows in canonical configurations such as uni- and bi-directional traffic in a hallway using the descision-based model developed in [1], and analyze the waves and turbulence that are known to develop under certain conditions. You will also carry out comparisons with experimental studies of pedestrian behavior and critically assess the strengths and weaknesses of the model and develop improvements as appropriate.

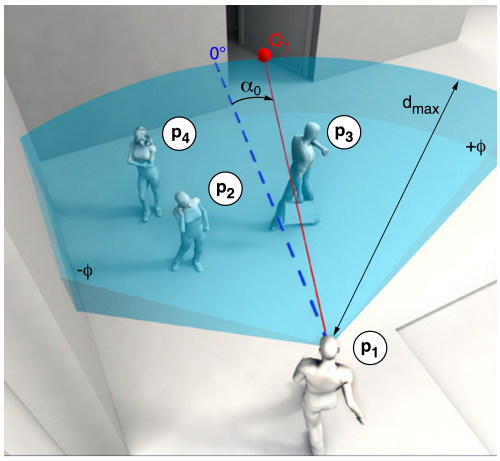


Illustration of a pedstrian (p_1) analyzing her path (taken from [1])

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 modeling of pedestrian behavior
· 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 Computation. Python programming experience will be helpful.

Reference

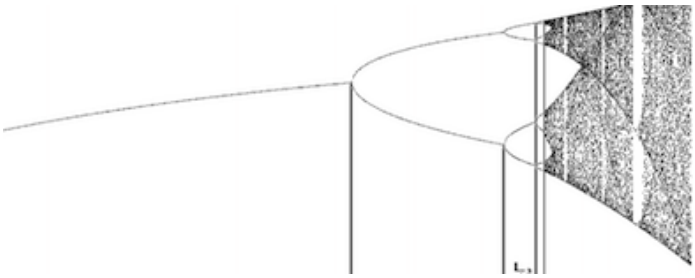
[1] M. Moussaid, D. Helbing, & G. Theraulaz. How simple rules determine pedestrian behavior and crowd disasters. Proc. Natl. Acad. Sci. USA, 108::6884-6888 2011.

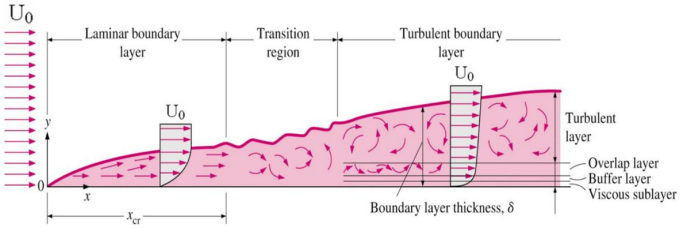
Transition to chaos in model spatially-developing flows

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-temporal 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.

MSc applied mathematics projects with Dr Vahid Shahrezaei

Project 1: Stochastic genetic networks and developmental robustness

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. Among all multicellular organisms, a simple worm, 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. This project is in close collaboration with biologists at Imperial and using their data on the developmental programs of this worm that we will combine with stochastic models of genetic networks to unravel mechanisms of developmental robustness.

Project 2: Machine learning approaches for efficient analysis and inference in complex biological models

Mathematical models encountered in real biological problems can be complex, high dimensional and slow to simulate. This poses many challenges to efficient exploration of these models across parameter space. Also, inference using likelihood free methods such as Approximate Bayesian Computation can be inefficient. In this project, we explore using different machine learning methods to assist in efficient analysis and inference for such models.

Dr Philipp Thomas - Stochastic processes in biology

Web: https://www.ma.imperial.ac.uk/~pthomas

PROJECT 1: **Trajectory inference methods for continuous-time Markov chains**

Supervisor: Dr Barbara Bravi (b.bravi@imperial.ac.uk), Dr Philipp Thomas (p.thomas@imperial.ac.uk)

Cellular reaction networks are inherently noisy. Understanding the sources of this variation is important since it affects many essential cell functions. The wealth of data generated by modern time-lapse microscopy requires sophisticated statistical inference tools to connect data with mechanistic models.

The chemical master equation models intracellular reactions as a continuous-time Markov chain. While inference tools for Markov chains are well developed, they do not immediately apply to stochastic reaction networks because the number of accessible states in these networks is, at least in principle, unbounded. The idea of this project is to combine the expectation-maximization algorithm with the Finite State Projection Algorithm (FSP) to find the unknown parameters of the network from noisy time-series data. The FSP algorithm is a finite-dimensional approximation of the master equation, providing error estimates and convergence guarantees that can inform the inference. You will probe the efficacy of the methodology using live cell microscopy data.

Literature:
Wikipedia - Baum-Welch Algorithm (https://en.wikipedia.org/wiki/Baum%E2%80%93Welch_algorithm)

Munsky et al (2006) *The finite state projection algorithm for the solution of the chemical master equation* J. Chem. Phys. 124, 04410 (https://aip.scitation.org/doi/10.1063/1.2145882)

PROJECT 2: **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, we will investigate solutions to age-structured population dynamics driven by environmental inputs. We will study the effects of age-dependent population growth dynamics using analytical and simulation-based methods. In particular, we will develop methods to quantify growth rates and age distributions, drawing from connections between point processes and survival analysis.

Interest in the analysis of stochastic processes is required.

Literature:

Inaba, H (2017). Age-structured population dynamics in demography and epidemiology (Chapter 1), Springer Book.

Aalen, Odd, Ornulf Borgan, and Hakon Gjessing (2008). *Survival and event history analysis: a process point of view*. Springer Book.

Martins, B. M., Tooke, A. K., Thomas, P., & Locke, J. C. (2018). Cell size control driven by the circadian clock and environment in cyanobacteria. *PNAS*, *115*, E11415-E11424.

MSc project proposals

Thesis Advisor: Benjamin Walter

November 25, 2022

Contact: b.walter@imperial.ac.uk

1 First return of N random walkers

1.1 Topic

One of the fundamental observations of statistical mechanics is that in equilibrium it is exceedingly unlikely to observe very ordered states. Considering a volume filled with an ideal gas, it is extremely rare that all atoms arrange on the, say, left half of the volume at the same time. But what about the non-equilibrium scenario? We will study the following toy model: a one-dimensional volume, $[-L, L]$, is divided by a tiny wall into a left and a right chamber ($[L, 0)$ and $(0, L]$). The left chamber is filled with N atoms which are modelled as non-interacting Brownian motions, while the right one remains empty. At time $t = 0$, we remove the wall. How long does one need to wait to *first* see all N walkers return into the left chamber?

This problem is related to *first-passage times*, a key question of non-equilibrium statistical physics which asks for the *first* time a certain event is observed. Although seemingly simple, already the one-dimensional system has some intriguing features which clearly illustrate the difference between equilibrium and non-equilibrium statistical physics.

In this project, we'll explore stochastic dynamics of simple systems out of equilibrium, and study how *rare events* can be treated analytically to reveal deep insights into the relaxation towards an equilibrium state.

1.2 Features

Suited for students who are interested in: Stochastic processes, foundations of statistical mechanics, analysis and combinatorics.

Analytical techniques that will be learned on the way: Path integrals, saddle point approximations, Laplace transforms, large deviation functions, integral transforms, as well as some advanced numerical methods to sample rare events.

Helpful skills: Integrating by hand, programming in a fast language (C, Julia or similar)

2 Extreme events of a quantum random walk

2.1 Topic

In classical statistical physics, the random walker is a particle which lives on a lattice (for instance $\mathbb{Z}$) and which in each time step randomly hops either onto the left or right neighbouring site with equal probability. It is a well studied model with many applications and a long standing research tradition.

More recently, people started to study its quantum analogy, the quantum random walk. A quantum random walker *simultaneously* explores all possible paths, but these paths interfere with each other, leading to surprising and bizarre physics. In this project, we will investigate a number of *extreme events* such as the likelihood to measure the particle at an atypically far distance, or the *first* time a particle is detected at a given site. However, as it's a quantum particle, the very act of measuring a position affects the entire evolution...

In this project, we explore the competition between the unitary evolution of a quantum particle and repeated quantum measurements, and how it can be seen through the lens of extreme events.

2.2 Features

This project is suited for students who are interested in quantum mechanics, probability, and (non-equilibrium) statistical physics. We will get to know various analytical techniques such as renewal equations, z transforms, generating functions and complex integration. Some prior experience with linear algebra, complex analysis, and scientific computing will be useful.

3 From continued fractions to the disordered Schrödinger equation

3.1 Topic

A continued fraction is a number z that is given by an infinite sequence of $a_0, a_1, \ldots$ via

$$z = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \ldots}}}. \tag{1}$$

If the $a_i's$ are drawn as independent and identically distributed random variables from some distribution $p(a)$, what is the probabiltiy distribution of z? For instance, if the a_i's are chosen randomly to be $+1$ or -1, how would z be distributed?

It turns out that these seemingly innocent questions are not only hard to answer but also have deep connections to the behaviour of a quantum particle in a randomly disordered (=rugged) potential, or, for the more mathematically inclined, random dynamical systems and random matrix theory.

In this project, we will study the distribution of z for some simple distributions of a, and then apply our findings to the so-called binary alloy model, a model for disordered crystals.

3.2 Features

This project is suited for students interested in unexpected connections between random dynamical systems, linear algebra, disorder and randomness, fractals, and quantum mechanics. It involves a mix of analytical and numerical work, so prior experience with scientific computing is particularly helpful. The tools we will get to know are random matrix theory, ordinary differential equations, integral equations, and numerical schemes to solve them.

Nonlinear dynamics of vortices on axisymmetric shear flows (**Prof. X. Wu**)

Axisymmetric shear flows arise in technology as well as in nature. Two well-known and representative examples are the circular jets, which are used in high-speed propulsion, and tropical cyclones, which characterise hurricanes and typhoons. Typically, an axisymmetric shear flow field consists of both axial and azimuthal velocities, but the limiting cases of pure axial and azimuthal motions are of interest also.

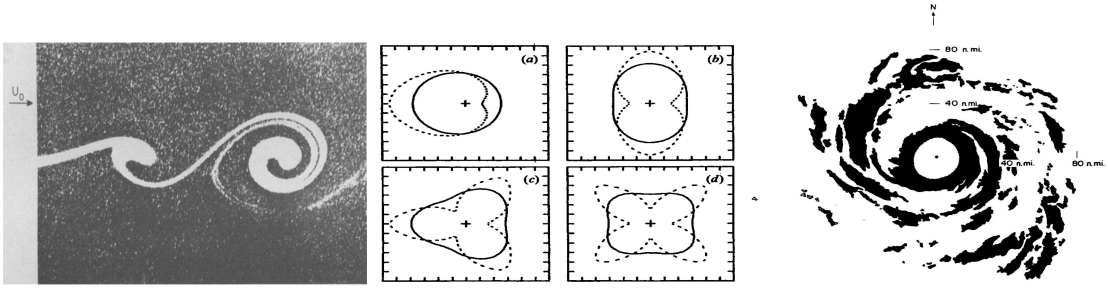


Figure 1: Left: Vortex of a ring mode on a circular jet, a cross-section view on the plane through the jet axis. Middle: loss of axisymmetry shown by the mean-flow axial velocity contours in plane perpendicular to the axis. Right: Spiral bands in a hurricane.

Circular jets, in which the axial motion is dominant, have been extensively studied because of their importance in technology. Such a flow is unstable, and as a result unsteady perturbations with frequencies in a certain band amplify in their intensity (Cohen & Wygnanski 1987), leading to formation of vortices (see the left figure). Linear stability theory predicts that amplifying perturbations may be axisymmetric and non-axisymmetric, which are referred to as ring modes and helical modes, respectively. These modes co-exist and are independent of each other when their amplitudes are sufficiently small. However, once all or some of the modes have reached a threshold intensity, mutual as well as self nonlinear interactions take place, causing the resultant vortices to exhibit rich temporal and spatial dynamics. One of the interesting features observed in experiments is *vortex pairing*: two adjacent vortices merge as they develop. This is attributed to the nonlinear interaction between a dominant mode and its subharmonic component (Zaman & Hussain 1980). Another interesting behaviour is that although the mean jet flow is axisymmetric initially, it becomes non-axisymmetric downstream (see the middle figure). It has been suggested the mechanism is due to the mutual interaction between helical modes with (nearly) the same frequency (Wu 2019). As these dynamical behaviours are closely related to emission of jet noise, in this project we will develop appropriate mathematical theories to describe and predict the observations.

An axisymmetric shear flow with a dominating swirling (azimuthal) velocity resembles the primary flow field of a tropical cyclone. A hallmark of the latter is the system of spiral bands (see figure 1c), which are related to rainstorms in a cyclone. The formation of the bands has not been fully explained. A possible mechanism is associated with the instability of the underlying flow field (Lewekw, Le Dizes & Williamson 2016). An investigation of this possibility is another direction (or aim) of this project. Specifically, we would like to develop a theory describing the initiation, intensification and subsequent attenuation of the spiral bands. Furthermore, complex dynamics within the bands, such as wave breaking, may also be captured by theory.

This project involves mathematical analysis (using asymptotic techniques) and numerical computation, with the weight for each being dependent on the interest of the

student.

References:

1. Zaman, K. B. & Hussain F. 1980 Vortex pairing in a circular jet under controlled excitation. Part 1. General jet response. *J. Fluid Mech.* **101**, 449-491.

2. Cohen, J. & Wygnanski, I. 1987 The evolution of instabilities in the axisymmetric jet. Part 1. The linear growth of disturbances near the nozzle. *J. Fluid Mech.* **176**, 191-219.

3. Wu, X. 2019 Nonlinear theories for shear-flow instabilities: physical insights and practical implications. *Annu. Rev. Fluid Mech.* **51**, 421-485.

4. Leweke, T., Le Dizes, S. & Williamson, C. 2016 Dynamics and instabilities of vortex pairs. *Annu. Rev. Fluid Mech.* **48**, 507-541.

Modelling boundary-layer instabilities from a unified perspective of wall impedance (Prof. X. Wu)

Boundary-layer flows are common in nature and technological applications. The atmospheric flow near the Earth surface and the airflow near the surfaces of an aircraft and/or spacecraft are just two examples. Such flows may undergo transition from a simple laminar state to turbulence. Predicting this transition is of great importance because mixing, momentum exchange, drag and heat transfer in turbulent state are drastically different from those in its laminar counterpart.

Transition is associated with the intrinsic instabilities of the laminar boundary-layer flow, but is also crucially influenced by surface conditions, such as porous coating (lining) and roughness (Fedorov 2011). Different forms of instabilities may arise. Among them, inviscid instability is well understood thanks to calculations based on the vortex-sheet model as well as to Rayleigh's inflection point theorem, or the generalised inflection point theorem in the case of a compressible boundary layer. Much subtler and harder to understand is the mechanism of viscous instability, where viscous diffusion causes instability despite the fact that it dissipates the kinetic energy of the perturbation into heat. As the characteristic Reynolds number is large, viscous effects usually become important in the vicinity of the wall but negligible in the main bulk of the flow field. Interestingly, the effect of the viscous flow in this very thin sublayer on the inviscid part of the flow is shown to manifest as an *equivalent impedance coefficient*. For a distinguished band of frequencies, the impedance alters the phase relation in such a manner that instability arises. Compared with the standard description of triple deck theory, such an interpretation is more direct and has a clearer physical context. For other frequencies, viscous effects play a stabilising role. A theory based on the equivalent impedance was found to be mathematically simpler, computationally efficient and yet sufficiently accurate (Dong, Liu & Wu 2020).

Physical impedance effects could be generated by applying special lining or porous coating to the surface. In the case of supersonic boundary layers, appropriate coating has been found to inhibit the growth of the so-called second Mack mode (Fedorov 2011), which is the dominant instability, and transition may be delayed, bringing significant technological benefit.

Surface roughness usually enhances instability, causing earlier transition. However, certain form of roughness arrays, if carefully installed at right positions, may actually stabilise the boundary layer flow (Fujii 2006, Fransson *et al.* 2006). Interestingly, the effects of roughness could also be characterized as 'equivalent impedance'.

The present project will investigate the effects of different physical factors, including viscosity, surface roughness and porous coating, from the unified perspective of wall impedance. Using the technique of the so-called matched asymptotic expansion, the viscous flow in the thin sublayer adjacent to the wall will be analysed, pertinent to each, or a combination, of these factors to derive the equivalent impedance coefficient. The resulting models will be studied analytically and numerically to quantify the impact on linear and nonlinear instabilities. The models also enable us to study generation of sound waves, which is another physical aspect of importance.

References:

1. Dong, M., Liu, Y. & Wu, X. 2020 Receptivity of inviscid modes in supersonic boundary layers due to scattering of free-stream sound by localised wall roughness. *J. Fluid Mech.* **896**, A23.

2. Fedorov, A. V. 2011 Transition and stability of high-speed boundary layers. *Annu. Rev. Fluid Mech.* **43**, 79-95.

3. Fransson, J. H. M., Talamelli, A., Brandt, L. & Cossu, C. 2006 Delay transition to turbulence by a passive mechanism. *Phy. Rev. Lett.* **96**(6), 064501.

4. Fujii, K. 2006 Experiment of the two-dimensional roughness effect on hypersonic boundary-layer transition. *J. Spacecr. Rockets* **43** (4), 731-738.

The unsteady Kutta condition and excitation of instability modes in the wake flow (Prof. X. Wu)

When an object such as an aircraft moves through an ambient fluid, a wake forms downstream. A wake is usually unstable, which means that a small disturbance to the flow amplifies. The amplification leads to interesting and complex dynamics. The wake flow and the development of perturbations are important because they are related to the drag on the object, and in the case of aircraft taking off and landing, the wake downstream of one aircraft influences the flight of the next.

In order to investigate experimentally the instability of a wake, it is customary to produce a sound wave (using a loudspeaker) to excite an instability wave (mode) in a controlled manner so that the development of the latter can be studied in detail. This process, which is referred to as receptivity, is also an important part of aerodynamic noise generation.

Theoretical studies of instability and receptivity are usually based on inviscid approximation. The solution is however often non-unique, and an unsteady Kutta condition is then imposed in order to select the physically acceptable solution (Crighton 1985). This condition is supposed to account for the viscous effects operating in the vicinity of the trailing edge of the object. The appropriateness of this condition is not apparent, and its justification requires a detailed analysis of the viscous flow near the trailing edge. Orszag & Crow (1970) used the unsteady Kutta condition in their study of the effect of the edge on the instability itself, and a corresponding viscous analysis was performed by Daniels (1978). In these studies, the external forcing (e.g. the incident sound) is absent, that is, the receptivity was not considered. In the present project, we will investigate the receptivity, i.e. excitation of instability wave when a sound wave interacts with the edge. Both inviscid and viscous analyses will be performed using the matched asymptotic expansion as the mathematical tool, and the asymptotic matching between the inviscid (outer) and

viscous (inner) solutions would define and justify the Kutta conditions to be used. Moreover, we can determine the amplitude of the instability mode (eigen solution) in terms of the characteristics of the sound wave and the geometry of the edge.

This project is primarily analytical, involving a systematic analysis using the matched asymptotic expansion technique, but some numerical calculations are required in order to obtain the results of relevance for practical applications.

References:

1. D. G. Crighton 1985 The unsteady Kutta condition in unsteady flow. *Ann. Rev. Fluid Mech.* **17**, 411-445.

2. P. G. Daniels 1978 On unsteady Kutta condition. Q. J. Mech. Appl. Math. **31**, 49-75.

3. Orszag, S. A. & Crow, S. C. 1970 Instability of a vortex sheet leaving a semi-infinite plate. *Stud. Appl. Math.* **49**, 167-181.

Michele Coti Zelati: Mixing for Hamiltonian flows via action-angle coordinates

The goal of this project is to study the mixing properties of a passive scalar f that satisfies the transport equation

$$\partial_t f + \boldsymbol{u} \cdot \nabla f = 0, \tag{1}$$

where $\boldsymbol{u}$ is a given, time-independent and divergence-free velocity vector field on $\mathbb{T}^2 = [0, 2\pi)^2$. In this case, $\boldsymbol{u} = \nabla^\perp H = (-\partial_y H, \partial_x H)$, where $H : \mathbb{T}^2 \to \mathbb{R}$ is a regular Hamiltonian. Under certain conditions, the action-angle coordinates allow to transform the above equation (1) into an equation of the form

$$\partial_t f + \frac{1}{T(h)} \partial_\theta f = 0, \tag{2}$$

where $T(h)$ is the period of the closed orbit $\{H = h\}$, and $\theta \in [0, 2\pi)$ is the angle coordinate. Equation (2) can be studied through the stationary-phase method, and it is crucial to understand the properties of $T'(h)$ in order to understand the mixing properties of (2).

The goal of this project is two-fold: get familiar with the stationary phase method, that allows to prove decay of oscillatory integrals, and compute $T(h)$ for classical flows other than the one studied in [1].

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

References

[1] E. Bruè, M. Coti Zelati, and E. Marconi, *Enhanced dissipation for two-dimensional Hamiltonian flows*, arXiv e-prints (Nov. 2022), available at 2211.14057.

Michele Coti Zelati: Lyapunov Exponents for Markov Chains

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi^t(x) = u_t(\phi^t(x)), \qquad \phi^0(x) = x, \tag{1}$$

where 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

$$\partial_t g_t + u_t \cdot \nabla g_t = 0, \qquad g_0 = g, \tag{3}$$

via the formula $g_t = g \circ (\phi^t)^{-1}$. Many of these problems can be rephrased in terms of Markov chains, as done in [1]. The goal of this project is to find minimal condition for Markov chains to have a positive Lyapunov exponent, using variants of the classical Furstenberg criterion, and verify them through a combination of analytical and numerical techniques for particular velocity fields u.

Prerequisites. Students taking on this project are required to have some basic understanding of differential equations, random dynamical systems, Markov chains.

References

[1] A. Blumenthal, M. Coti Zelati, and R. S. Gvalani, *Exponential mixing for random dynamical systems and an example of Pierrehumbert*, arXiv e-prints (Apr. 2022), available at 2204.13651.

Zatorska, Ewelina

Title: Duality solutions for systems of conservation laws

Description: The Partial Differential Equations (PDEs) are often used to describe certain conservation laws in physics and in biology. The most well-known examples include conservation of mass, momentum and energy. The underlying equations can be solved separately but also as the systems of equations like the Euler or Navier-Stokes equations for fluids.

The students might be already familiar with the Burgers equation that is one of the simplest nonlinear PDEs describing convection. Even for this basic equation the classical solutions may develop shocks in finite time. To capture this behaviour, a more general notion of solution is necessary.

The goal of this project will be to prove existence of the so-called duality solutions to the pressure less degenerate compressible Navier-Stokes equations in one-dimensional domain.

The project will use elements of theory developed for pressureless Euler equations by

F. Bouchut and F. James:

- One-dimensional transport equations with discontinuous coefficients, NonlinearAnalysis 32 (1998), no. 7, 891,

-Duality solutions for pressureless gases, monotone scalar conservation laws, and uniqueness, Communications in PDEs 24 (1999), no. 11-12, 2173–2189.

The prerequisites for this project are the theory of Partial Differential Equations, and some elements of Analysis, Functional Analysis and Mearure Theory.

Section: Applied

Enriched finite element method for the Stokes equations

Supervisor: Abdalaziz Hamdan (supported by Colin Cotter)

Suitable for 1 student.

Description

This project focusses on computer implementation of a particular finite element method using the Firedrake library in Python (Firedrake, 2022).

Finite element discretisations for the Stokes equation of low Reynolds number fluid flow has been a challenge for decades, because of the difficulties of finding suitable cellwise polynomial representations (i.e., finite element spaces) for the velocity and pressure such that the discretisation is stable. In particular, there is a continued search for discretisations that have local mass conservation, which occurs when the pressure space is discontinuous. The classical example of the Scott-Vogelius element has continuous piecewise quadratic functions for velocity (P2) and discontinuous piecewise constant functions for pressure (P0) is partially successful in that it is stable, but only on certain meshes; also the rather high degree polynomials seems excessive for a first order method. Recently an alternative has been proposed, the Enriched Galerkin method (Yi et al., 2022), which uses continuous piecewise linear functions for velocity, enriched with some additional discontinuous functions for stability.

In this project we shall investigate suitable approaches to solve this equation using the Firedrake system, which allows the high level specification of finite element problems through code that looks like maths, which is then automatically translated by the system into high performance compiled code. This approach allows MSc project students to quickly develop and investigate different methods, since all the low level details are dealt with automatically. We will investigate the convergence of the scheme through numerical experiments, and explore the efficient scalable solution of the resulting matrix-vector systems through the block preconditioning proposed in the paper. If there is time, we will investigate efficient multigrid methods for this system as well.

References

Firedrake, 2022. The firedrake website. `https://firedrakeproject.org`.

Yi, S.Y., Hu, X., Lee, S., Adler, J.H., 2022. An enriched galerkin method for the stokes equations. Computers & Mathematics with Applications 120, 115–131.

Section: Applied

Time-parallel solution of optimal control problems for the wave equation

Supervisor: Abdalaziz Hamdan (supported by Colin Cotter)

Suitable for 1 student.

Description

This project focusses on computer implementation of a particular finite element method using the Firedrake library in Python (Firedrake, 2022).

Optimal control problems seek to provide forcing for a dynamical system that guides the solution towards a chosen trajectory whilst minimising some chosen cost function. These are challenging problems since they require the optimal forcing to be solved for all times simultaneously. Gander et al. (2020) proposed a solution strategy for this problem (in the case of quadratic cost) based on a new type of "paradiag" preconditioner that block diagonalises the system using fast Fourier transform in time, resulting in independent systems to be solved for each time.

In this project we shall investigate suitable approaches to solve this equation using the Firedrake system (focussing initially on 1D in space), which allows the high level specification of finite element problems through code that looks like maths, which is then automatically translated by the system into high performance compiled code. This approach allows MSc project students to quickly develop and investigate different methods, since all the low level details are dealt with automatically. We will investigate the convergence of the scheme through numerical experiments, and, if time, will explore the extension of this scheme to mixed formulations of the wave equation which use first order systems of equations instead of a single second order system (this allows to bridge the gap to fluids and Maxwell's equations).

References

Firedrake, 2022. The firedrake website. `https://firedrakeproject.org`.

Gander, M.J., Liu, J., Wu, S.L., Yue, X., Zhou, T., 2020. Paradiag: Parallel-in-time algorithms based on the diagonalization technique. arXiv preprint arXiv:2005.09158 .

NEURAL AVALANCHE CORRELATIONS IN ALTERED STATES OF CONSCIOUSNESS

Hardik Rajpal
Department of Mathematics
h.rajpal15@imperial.ac.uk

Pedro A.M. Mediano
Department of Computing
pedro.martinez-mediano13@imperial.ac.uk

Henrik Jeldtoft Jensen
Department of Mathematics
h.jensen@imperial.ac.uk

ABSTRACT

Cascades of neural avalanches detected in cortical MEG and EEG recordings of humans exhibit amplification-attenuation dynamics (AAD) which correlates well with the prevalence of alpha rhythms in the human brain activity. These cascades show long and short term temporal correlations that provide some insight into human cognitive behaviour. In a recent paperLombardi et al. (2022) it was discussed that such long and short-term AAD regulation of brain activity was absent in non-REM sleep states in human subjects. The proposed study wishes to extended this analysis to altered states of consciousness where these alpha-rhythms are suppressed in states induced by certain psychedelics in resting state. Thus allowing us to disentangle the role of AAD in states of high cognition where alpha waves are suppressed.

1 INTRODUCTION

Cortical brain oscillations have been observed and extensively studied in various neuroimaging studies. However a dynamical and mechanistic explaination of their emergence is still lacking. In order to further explore the mechanisms through which these waves may regulate human cognition various studies based on neural avalanches have been publishedLombardi et al. (2014; 2016; 2021); Nandi et al. (2022). Most recentlyLombardi et al. (2022), it was identified that avalanche size changes among neighbouring avalanches $\Delta s = s_{i+1} - s_i$ (where s_i denotes size of the avalanches), when compared with the quiet times follow a characteristic attenuation-amplification behaviour around the 100ms timescale corresponding to the alpha waves. Interestingly, this characteristic behaviour was found to be absent in subjects in the Non-REM (NREM) sleep. Thus, making this mechanism closely related to the presence of alpha waves in these two cognitively different states.

However, there can be states with increased cognition where alpha activity is suppressed. Deploying the above mentioned avalanche analysis on such states can help clarify the role of this AAD mechanism as a cognitive mechanism. The resting state MEG datasets of subjects in placebo as well as psychedelic states provide an ideal set-up to perform this analysis.

2 PROPOSED STUDY

It has been well known that psychedelics suppress alpha wave power among mice and animal studiesHolmes & Korteling (1993); Lozano-Soldevilla (2018); Jinks (2019).Simultaneously, subjects in these states repored increased awareness, visual hallucinations and emotional experiences. This

state is vastly different from states with low alpha and lower cognition like the NREM sleep state mentioned above.

By replicating the avalanche size and quiet time probability distributions on the resting state MEG data from LSD, KET and Psilocybin subjects and comparing that to placebo trials, we can further comment on the role of amplification-attenuation dynamics as necessary for cognition or as a signature of alpha waves in human brains.

3 PREREQUISITES

ESSENTIAL

- Strong background in programming (Python/ Matlab).
- Some experience in working with neuroimaging datasets (fMRI/MEG/EEG) and preprocessing.

DESIRABLE

- Background in theory of self organized criticality and avalanches.

REFERENCES

Gregory L Holmes and Faye Korteling. Drug effects on the human eeg. *American Journal of EEG Technology*, 33(1):1–26, 1993.

Tony Jinks. The how and why of psychedelics. In *Psychological Perspectives on Reality, Consciousness and Paranormal Experience*, pp. 179–190. Springer, 2019.

Fabrizio Lombardi, Hans J Herrmann, Dietmar Plenz, and Lucilla De Arcangelis. On the temporal organization of neuronal avalanches. *Frontiers in systems neuroscience*, 8:204, 2014.

Fabrizio Lombardi, Hans J Herrmann, Dietmar Plenz, and Lucilla De Arcangelis. Temporal correlations in neuronal avalanche occurrence. *Scientific reports*, 6(1):1–12, 2016.

Fabrizio Lombardi, Oren Shriki, Hans J Herrmann, and Lucilla de Arcangelis. Long-range temporal correlations in the broadband resting state activity of the human brain revealed by neuronal avalanches. *Neurocomputing*, 461:657–666, 2021.

Fabrizio Lombardi, Hans J Herrmann, Liborio Parrino, Dietmar Plenz, Silvia Scarpetta, Anna Elisabetta Vaudano, Lucilla de Arcangelis, and Oren Shriki. Alpha rhythm induces attenuation-amplification dynamics in neural activity cascades. *bioRxiv*, 2022.

Diego Lozano-Soldevilla. On the physiological modulation and potential mechanisms underlying parieto-occipital alpha oscillations. *Frontiers in computational neuroscience*, 12:23, 2018.

Manoj Kumar Nandi, Alessandro Sarracino, Hans J Herrmann, and Lucilla de Arcangelis. Scaling of avalanche shape and activity power spectrum in neuronal networks. *Physical Review E*, 106 (2):024304, 2022.

INFORMATION PROCESSING AT ORDER-DISORDER PHASE TRANSITIONS

Hardik Rajpal
Department of Mathematics
h.rajpal15@imperial.ac.uk

Henrik Jeldtoft Jensen
Department of Mathematics
h.jensen@imperial.ac.uk

ABSTRACT

Complex systems are known to exhibit interesting information processing capabilities near critical transitions. For instance measures like information storage and transfer peak near critical transitions in 2D Ising model as well as Random Boolean Networks near the critical values of order parameter. However, it is less clear how these information measures differ in their behaviour at the transition between continuous and discontinuous phase transitions. This project aims at using Potts model to compare and contrast the various information theoretic measures for different values of possible spins q that dictate the continuity of phase transition in the model.

1 INTRODUCTION

In recent years information theory has become a powerful tool to study complex systems, especially from the point of view of information processing. This has lead to an alternative understanding of traditional complex systems with the language from communication and signal processing. Different parts of the system can store, transfer and collectively modify information as part of they evolve together.

These interactions can be quantified using various information measures such as active information storage, transfer entropy, interaction information etc. Applications of these information measures on existing models of statistical mechanics has revealed some interesting properties of the critical state. It has been shown for the 2D ising modelBarnett et al. (2013), Random Boolean NetworksLizier et al. (2008), cellular automataLizier (2014) and kuramoto oscillatorsMediano et al. (2022). All of these applications show a peaking behaviour of information measures when the parameter of the dynamics are tuned close to critical behaviour. This description of the critical state has enhanced our understanding of why so many socio-economicBossomaier et al. (2013) and livingTkačik & Bialek (2016) systems self-organize near the critical point.

The proposed study wishes to extend these results to study characteristic differences between the continuous and discontinuous phase transitions. This is indeed inspired by to verify if the peaking behaviour is characteristic of critical systems or order-disorder transitions in general. Supplementing the information-theoretic analysis with knowledge from statistical mechanics is key to further our understanding of information-processing near phase transitions.

2 PROPOSED STUDY

Potts modelPotts (1952) is a generalized ising model of order-disorder transitions where every spin can take q different values. Interestingly, it has been shown that the model exhibits continuous first order transitions for $q > 4$ and discontinuous phase-transitions for $q \leq 4$. The model converges to the 2d ising model for $q = 2$.

The model thus provides an ideal setup for comparing in contrast the information processing near phase transitions for different values of q and thus the continuity of transitions.

3 PREREQUISITES

ESSENTIAL

- Strong background in programming (Python/ Matlab/ C++ or any other OOP language).
- Background in statistical mechanics of phase transitions

DESIRABLE

- Background in information theory and estimating information-theoretic measures.
- Modelling and simulation of spin systems

REFERENCES

Lionel Barnett, Joseph T Lizier, Michael Harré, Anil K Seth, and Terry Bossomaier. Information flow in a kinetic ising model peaks in the disordered phase. *Physical review letters*, 111(17): 177203, 2013.

Terry Bossomaier, Lionel Barnett, and Michael Harré. Information and phase transitions in socio-economic systems. *Complex Adaptive Systems Modeling*, 1(1):1–25, 2013.

Joseph T Lizier. Measuring the dynamics of information processing on a local scale in time and space. In *Directed information measures in neuroscience*, pp. 161–193. Springer, 2014.

Joseph T Lizier, Mikhail Prokopenko, and Albert Y Zomaya. The information dynamics of phase transitions in random boolean networks. In *ALIFE*, pp. 374–381. Citeseer, 2008.

Pedro AM Mediano, Fernando E Rosas, Juan Carlos Farah, Murray Shanahan, Daniel Bor, and Adam B Barrett. Integrated information as a common signature of dynamical and information-processing complexity. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 32(1):013115, 2022.

Renfrey Burnard Potts. Some generalized order-disorder transformations. In *Mathematical proceedings of the cambridge philosophical society*, volume 48, pp. 106–109. Cambridge University Press, 1952.

Gašper Tkačik and William Bialek. Information processing in living systems. *Annual Review of Condensed Matter Physics*, 7:89–117, 2016.