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maximising impact through mathematics

Monash Academy for Cross &
Interdisciplinary Mathematical Applications

MAXIMA Mathematical Interdisciplinary PhD Projects

Table of Projects

Understanding the origins of aneuploidy in cell division using mathematics

Supervisors

* Dr Mark Flegg (MAXIMA, School of Mathematical Sciences)
Prof. John Carroll (Faculty of Biomedical and Psychological Sciences)

*Email: mark.flegg@monash.edu

Background

Aneuploidy is a genetic abnormality whereby an abnormal number of chromosomes are present in a cell often caused by errors in the attachment of microtubules (MT) to the kinetochores (KT) during the metaphase stage of the cell cycle. Clarifying the origins of this abnormality is crucial to understanding conditions such as cancer and genetic developmental disorders such as Down Syndrome.

In this project we will use mathematical and statistical approaches to elucidate the effect of age-dependent kinetochore separation during the cell cycle on the frequency of KT-MT attachment errors. We will develop a mechanistic mathematical model of aneuploidy which will involve the effect of known chemical effectors and mechanical considerations. We will use Bayesian inference methods to ensure parameters of the model are fitted to experimental data.

Additional relevant information

Students will apply for an APA scholarship, $26,288 per annum (2016 rate). A top-up scholarship of $5000 per annum is available to exceptional applicants. There is also some start up project funds that may be used to support a suitable student.

Cancer Systems Biology

Supervisors

Dr Lan Nguyen (Department of Biochemistry and Molecular Biology)
A/Prof Tianhai Tian (School of Mathematical Sciences)

Email: Lan.K.Nguyen@monash.edu

Background

The Integrated Network Modelling Laboratory led by Dr Lan Nguyen at the School of Biomedical Sciences and Biomedical Discovery Institute, Monash University is seeking outstanding and enthusiastic candidates to carry out PhD study in cancer systems biology with a focus on network-level modelling of cancer signal transduction networks.

Dr Nguyen's lab is employing highly interdisciplinary approaches that combine mathematical modelling and systems analysis with cutting-edge experimental techniques in biochemistry and cell biology to investigate emergent properties and dynamic behaviour of signalling networks in normal and cancerous cells. These tools allow us to elucidate how and when cells make specific cell-fate decisions. Importantly, we utilise this knowledge to understand how resistance to targeted drugs come about and to derive new therapeutic strategies that can overcome network-encoded drug resistance.

A multitude of computational methods including (but not limited to) deterministic ordinary differential equations (ODEs), stochastic modelling, rule-based simulations and experimental techniques including proteomics, biochemistry-based assays and imaging will be integrated to develop quantitative and predictive models of these networks in normal and disease contexts. Prospect candidates who are to work on available projects will collaborate with biologists and benefit greatly from a highly interdisciplinary and stimulating environment in the Lab by interacting on a daily basis with researchers with both dry and wet expertise.

Students with a strong computational background with an interest in biology/cancer research are invited to apply for the positions. A variety of projects for Honours and MSc are also available in the Lab.

Additional Relevant Information:

$AUD 26,228 per annum full-time rate (tax-free stipend for 3 years, with possible 6 months extension)

Recommended reading/viewing:

Lab website: http://www.med.monash.edu.au/biochem/staff/lan-nguyen.html

Mathematical modelling of cell signalling pathway using proteomic data

Supervisor

* A. Prof. Tianhai Tian (School of Mathematical Sciences)

*Email: tianhai.tian@monash.edu

Background

The advances in proteomics technologies offer an unprecedented opportunity and valuable resources to understand how living organisms execute necessary functions at systems levels. However, it is still a significant challenge to utilize the highly accurate spatio-temporal dynamic proteome data for mathematical modeling of complex cell signaling pathways. Using the MAP kinase pathway as the test system, this project will design novel computational framework to develop mathematical models based on proteomic datasets. We will also design effective statistical inference methods to estimate unknown parameters in the model using proteomic and other experimental data.

Additional relevant information

Contact Tian for details.

Neuroscience

Supervisors

Prof Ramesh Rajan (Department of Physiology)
Prof Kate Smith-Miles (School of Mathematical Sciences)

Email: ramesh.rajan@monash.edu

Background

Neuronal responses are variable in all areas of the brain. Thus, in a typical experiment conducted on understanding how we gain information about the world through our senses, a neuroscientist would study a specific brain area devoted to processing information in that sensory in a sensory area (say a specific visual or auditory or tactile processing area of the cortex of the brain) and record the electrical activity from many neurons in that area, using specific sensory stimuli. This procedure would be repeated (or conducted) in a number of individual neurons in different layers of the sensory cortex (each layer carries out a different function, from being the input or integrative or output layers). Each neuron would be tested with a suite of different stimuli with appropriate variables of interest (motion direction, surface texture, voice pitch etc). Each stimulus would be repeated many times and average responses used to characterise that neuron's responses to the stimulus. From these sorts of procedures, we then infer how neurons in different layers of that specific area encode (signal) that stimulus.

We are interested in developing more sophisticated mathematical approaches to studying how sensory cortex neurons encode information about the world. Now, using a very large data base that we have already collected from the touch sensitive areas of the rat brain, we wish to determine the response statistics of different individual neurons, in the different layers, to the different stimuli and how these are affected after brain injury cases. Specifically, we wish to determine:

(a) How efficiently do neural responses represent a stimulus? i.e., how many trials is needed for a faithful and reliable representation by neural responses of the stimulus, and how does this depend on the type of statistical criterion applied?
(b) Do neurons need to build up response probabilities through repetition or priming?
(c) Do the response statistics vary between different neurons in the different layers (are some layers more robust in representing the world reliably than other layers)?
(d) Do response statistics vary with the type of stimulus - simple vs varying complexity, and different stimulus strengths (amplitude)?
(e) How are these statistics altered in brain injury? ie. does a change in response statistics underlie the deficits seen in humans with brain injury?

Recommended reading/viewing:

Gergo Orban, Pietro Berkes, Jozsef Fiser,& Mate´ Lengyel1 (2016) Neural Variability and Sampling-Based Probabilistic Representations in the Visual Cortex. *Neuron* 92, 530-543.

Network models of the human brain in health and disease

Supervisors

*A/Prof. Alex Fornito (Monash Institute for Clinical and Cognitive Neurosciences, MICCN).
Dr Ben D Fulcher (MICCN).
*Professor Kate Smith-Miles (MAXIMA and the School of Mathematical Sciences)

*Email: alex.fornito@monash.edu; kate.smith-miles@monash.edu

Background

The human brain is an extraordinarily complex network, comprising billions of nerve cells linked by trillions of fibers. The recent availability of high-quality datasets, acquired in species ranging from the nematode worm *C elegans* to the human, and spanning scales ranging from the micro to macro, has provided unpredicted opportunities for mapping and modelling the network architecture of nervous systems. In particular, the application of graph theory and complex systems analysis has revolutionized our understanding of structural constraints on brain network organization, their dynamical consequences, and the implications of both for disease. Advances in this field critically depend on: (1) the development and application of mathematical and statistical measures of network organization; (2) novel algorithms for modeling brain network organization, development and degeneration in disease; and (3) the identification of neurobiologically plausible measures of brain network topology.

We currently seek outstanding PhD candidates to conduct research into each of these areas. Candidates will have access to Monash University's world-class supercomputing facilities (e.g., MASSIVE), research dedicated brain-imaging equipment at Monash Biomedical Imaging, and large databases of magnetic resonance imaging data maintained at Monash Clinical and Imaging Neuroscience. This infrastructure provides a unique, integrated platform for the development and clinical application of novel methods and models characterising brain network structure and function, and enables seamless transition between theory and experiment.

Potential projects include:

- Developing novel statistical measures for measuring statistical dependencies in physiological time series data;
- Modelling how trade-offs between spatial, physical and functional constraints drive brain network development and evolution;
- Generative modelling of brain network development and degeneration;
- Modelling disease spread and communication processes on brain networks; and
- Biophysical modelling of brain network dynamics; and
- Relating simulated dynamics on structural brain networks to spatial maps of gene expression across the brain.

Additional relevant information

Joint supervision from the School of Mathematical Sciences, Monash Biomedical Imaging and the School of Psychology and Psychiatry, with a top-up scholarship available.

Highly comparative time-series analysis for diagnosis of brain disease

Supervisors

* Dr Ben D. Fulcher (MICCN)
A. Prof. Alex Fornito (MICCN)
Prof. Kate Smith-Miles (MAXIMA and School of Mathematical Sciences)

*Email: ben.fulcher@monash.edu

Background

Developments in brain imaging have allowed us to measure brain activity in humans non-invasively in health and disease, from the fast temporal resolution of brain dynamics measured using EEG, to the high spatial resolution of fMRI. These high-quality datasets are frequently measured to understand differences between patients with a brain disease (such as schizophrenia) and healthy controls, with the hope of developing brain-based biomarkers for diagnosis. These datasets are growing in size, and are increasingly being shared openly online.

Recently we have showed that regional differences in BOLD dynamics can be used to classify people with schizophrenia from healthy controls using a highly comparative approach to time-series analysis, a framework that allows comparison of thousands of scientific methods. In this project, the student will extend this work to look at different types of brain disorders, and apply new theory to investigate whether different brain diseases (including autism and major depressive disorder) represent extremes of healthy variation in the natural space of inter-individual variability. The results will provide new understanding on how different brain disorders manifest and are related to one another, and could lead to new biomarkers for diagnosis. Students should have an interest in the brain, large-scale numerical computations (on the Monash-based supercomputer, MASSIVE), and statistical machine learning algorithms.

Self-organisation of colon organoids

Supervisors

* Dr Mark Flegg (MAXIMA, School of Mathematical Sciences)
A. Prof. Helen Abud (Department of Anatomy & Developmental Biology)

*Email: mark.flegg@monash.edu

Background

Intestinal organoids are an exciting emerging technology in medicine. Intestinal crypt stem cells are grown in a lab. As the population of epithelium cells grow, they form spherical structures with multiple crypts in a very robust way (these structures are called organoids). Ingestion of the organoids find damaged areas of the intestine. The organoids deposit themselves to provide a new epithelial layer over damaged tissue. Despite the importance of this technology, how and why the organoids form crypts in the first place is unknown: there is no theoretical mechanism that is accepted by the biological community, despite experiments showing that chemicals are crucial components.

In this project we will explore possible theoretical mechanisms by which intestinal crypts spontaneously form as well as how one crypt may give rise to new crypts via budding. There are a number of different approaches that may be used to explore these mechanisms mathematically. PDEs describing signalling strengths and cellular populations along the axis of the crypt (or internally within the niche) can provide insight into dynamic changes that may occur in the crypt. Furthermore, it is likely that crypt budding is a result of an instability in the maintenance of a single crypt. Such instabilities can be explored analytically using PDE models. Simulation approaches to studying these phenomena may also be achievable such as cellular automata and/or the use of cell simulation packages such as CHASTE.

Additional relevant information

Students will apply for an APA scholarship, $26,288 per annum (2016 rate). A top-up scholarship of $5000 per annum is available to exceptional applicants.

Detecting non-protein coding RNAs contributing to cardiac function and development

Supervisors

*A/Prof. Jonathan Keith (School of Mathematical Sciences)
Dr Mirana Ramialison (Australian Regenerative Medicine Institute)
Dr Sarah Boyd (Clayton School of Info Technology)

*Email: jonathan.keith@monash.edu

Background

Bayesian change-point modelling is a statistical technique that can be used to detect interesting parts of biological sequences, including gene sequences. In this project, we will apply these methods to identify novel non-protein coding RNAs (ncRNAs) contributing to cardiac function and development.

Modelling mosquito populations to eliminate dengue

Supervisors

*A. Prof. Jonathan Keith (School of Mathematical Sciences)
Prof. Kate Smith-Miles (MAXIMA)

*Email: jonathan.keith@monash.edu

Background

Agent-based methods are used to model interactions between individuals in a population, with a high level of biological realism and fine spatio-temporal resolution. This project will apply Bayesian inference techniques to calibrate models of mosquito behaviour for the Eliminate Dengue Project, and optimisation techniques to identify optimal release strategies for reducing the ability of mosquitoes to transmit dengue.

Bayesian modelling of the spatio-temporal trajectory of antimalarial drug resistance

Supervisors

[1]A. Prof. Jonathan Keith (MAXIMA, School of Mathematical Sciences)
A. Prof. Manoj Gambhir (Epidemiology and Preventive Medicine)
Dr Jack Richards (Burnett Institute)

[1]Email: jonathan.keith@monash.edu

Background

Malaria is acknowledged as the most significant parasitic disease of humans in terms of global distribution and annual mortality. Artemisinin derivatives are the current frontline treatment of the disease, however a resistant strain has emerged along the Thailand-Myanmar border and in western Cambodia. Eliminating or containing the spread of this resistant strain is essential to ensure the continued global effectiveness of the best available treatment.
This project will develop, extend, evaluate and compare statistical and mathematical models of the spread of artemisinin resistance, and methods for inferring the structure and parameters of such models. The models and methods will be assessed for their usefulness in computationally simulating the spread of artemisinin resistance under a variety of management strategies, and identification of optimal strategies. An existing agent-based, spatio-temporal Bayesian model that has been used to model the spread of an invasive ant species in Australia will be modified and extended to model the spread of artemisinin resistance.

Additional relevant information

Students will apply for an APA scholarship, $26,288 per annum (2016 rate). A top-up scholarship of $5000 per annum is available to exceptional applicants.

Modelling Social Spreading Processes on Random Spatial Networks

Supervisors

[1]Prof. Hans De Sterck (School of Mathematical Sciences, Monash University)
[2]Dr. Joel Miller (School of Mathematical Sciences and School of Biological Sciences, Monash University)

[1]Email: hans.desterck@monash.edu
[2]Email: joel.miller@monash.edu

Background

It is intuitively clear that spatial structure influences key aspects of spreading processes on graphs and networks. For example, the connectivity of the neurons in our brains has a spatial structure that is essential for its functioning. Similarly, physical distance is an important factor in the social networks on which diseases, habits, fashions or beliefs propagate. Spreading processes on networks are often investigated theoretically using random graph models, but until very recently these models have neglected spatial structure.

In this project you will develop theoretical and computational models for spreading processes on new classes of random networks that intrinsically incorporate spatial structure. For example, we can consider population density and travel network data to construct random networks that model how populations interact inside and between cities, rural areas, and regions and countries further away, and how that may influence the spread of infectious diseases (think Zika, or Ebola), or social spreading processes such as obesity, or civil unrest.

The mathematical tools used and developed in this project include fast algorithms to generate random networks, stochastic simulation on networks, the derivation and analysis of differential equation models for spreading processes, and numerical solution techniques for these models.

There are many exciting developments in the field of complex networks research, and this project will allow you to contribute new knowledge at the leading edge to areas that are societally highly relevant. In particular, the project will encourage you to interact with researchers in areas such as public health and the social sciences to inform the research and help identify and answer some of the pressing questions in those fields.

Additional relevant information

A top up scholarship may be available for excellent candidates.

Large-scale computational modelling of epidemics in Australia: analysis, prediction and mitigation

Supervisors

[1]A. Prof. Manoj Gambhir (Epidemiology and Preventive Medicine)
Prof. Mikhail Prokopenko (University of Sydney)

[1]Email: manoj.gambhir@monash.edu

Background

This project brings the distinct perspective and power of network dynamics to resolve the problem of pathogen transmission, with a view to interruption. It will produce a computational framework specifically tailored for Australia. We will develop a national-level individual-based epidemiological model of the entire population of Australia, stochastically matching the most recent Australian Census data - Australia's 17th national Census will be held in August 2016, making this project very timely. The simulation approach will be grounded in real but anonymous data, both in terms of real population data (Census) and real disease surveillance data. This model will be combined with a novel network-theoretic and information-theoretic approaches, computationally tracing the epidemics within the simulated contact network, in order to predict crucial epidemic dynamics and formulate effective mitigation strategies. Thus, the "zooming in" capability will be further enhanced by an increased predictability of epidemic dynamics, in terms of infection rates, turning points, peaks and other critical variables. This furthermore will provide valuable inputs to estimation and advance planning of required resources, such as hospital beds, vaccinations, transport, and so on.

Additional relevant information

Students will apply for a PhD scholarship that has been funded by the ARC

Developmental and macroevolutionary controls of animal proportions

Supervisors[1]Dr Alistair Evans **(**School of Biological Sciences)
[1]Email: alistair.evans@monash.edu

Background

What are the rules for building an animal? Certain repeating elements of the body, such as teeth, fingers, limbs and vertebrae, are shown to follow the rule that the central element of three is the average size of the two elements each side. This simple rule constrains how the relative sizes of structures develop in the embryo and evolve over long periods of time. It is very influential in the evolution of tooth size in humans and our closest relatives (Evans et al. 2016, *Nature*). The precise mechanisms that determine the number and size of repeating structures, such as fingers and teeth, remain largely unknown.
This project aims to develop mathematical and computational models to investigate possible biological mechanisms of sequentially patterned growth. These models will be based on state-of-the-art experiments conducted at the School of Biological Sciences manipulating embryo development. Mathematical developments will involve reaction–diffusion problems on growing domains and generalisations of Turing-like patterning mechanisms.

Students with applied mathematics background and interest in developmental biology are strongly encouraged to apply. The prospective candidate will work closely with biologists and applied mathematicians in a stimulating interdisciplinary environment.

Additional relevant information

A scholarship top-up of up to $10,000 pa may be available for outstanding candidates who already hold an APA or equivalent scholarship.

Recommended reading/viewing:

Alistair Evans' Lab website: http://evomorph.org
Evans AR, Daly ES, Catlett KK, Paul KS, King SJ, Skinner MM, Nesse HP, Hublin J-J, Townsend GC, Schwartz GT, and Jernvall J. 2016. A simple rule governs the evolution and development of hominin tooth size. *Nature* **530**:477–480.
Kavanagh KD, Evans AR, and Jernvall J. 2007. Predicting evolutionary patterns of mammalian teeth from development. *Nature* **449**:427–432.
Turing AM 1952. The chemical basis of morphogenesis. *Phil. Transact. Royal Soc. B* **237**:37–72

Enhanced modelling of the behaviour of expansive soils

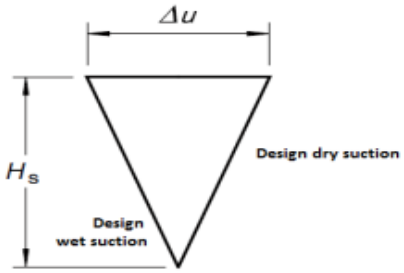
Supervisors

[1]Dr Jerome Droniou (School of Mathematical Sciences, Monash University)
[2]Dr Srikanth Venkatesan (School of Civil, Environmental and Chemical Engineering, RMIT)

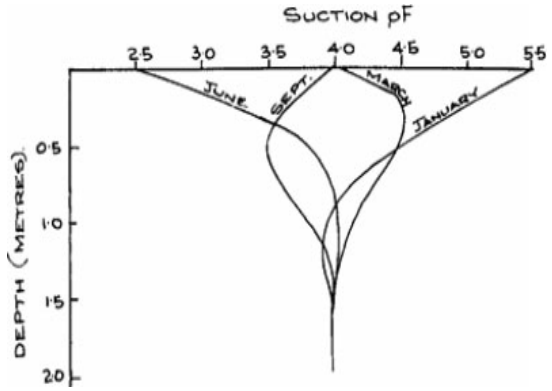
[1]Email: jerome.droniou@monash.edu
[2]Email: srikanth.venkatesan@rmit.edu.au

Background

Expansive soils correspond to soils whose volume can change in reaction to variation of their water content. This volume increases when the soil becomes wet, and decreases in dry seasons. Such changes provoke variations of the ground's height, possibly damaging structures built on top of it. Australian construction codes recommend an equation for soil movement that is based on the variations of soil suction. Suction is the key parameter which is defined as the ability to suck water from the soil (moisture flows from low suction to high suction regions). Widely used current models assume a triangular shape for the suction, fixing its value when deep underground and assuming a certain (more or less) fixed variation range at the ground level.
In practice, suction profiles are not triangular, but assume much more complicated shapes due to various environmental effects (climate, vegetation, etc.). See figure below.



In this project we aim at developing a more accurate model of suction, and to design a numerical scheme to compute approximate solutions for this model. Starting from 1D analysis, the goal of the project is to reach a complete 3D model that tackles both the fitting of parameters of interest and the prediction of suction values.



Topics in solar physics

Supervisors

Dr Alina Donea (School of Mathematical Sciences)

Email: alina.donea@monash.edu

Background

The Sun is a humming ball of sound waves launched by turbulent convective motions in our star's outer layers.

Because the sound speed beneath active regions is a bit faster than other places and because the reflecting layer beneath active regions is a bit deeper than other places, waves that include an active region at one of their bounce places will return to the front side a bit sooner than other waves.

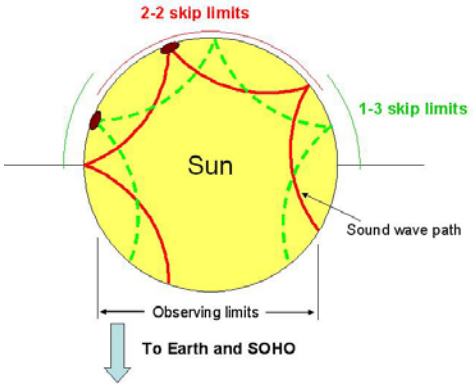


Figure 1 Illustrations of the two-skip measurement schemes used in the far-side imaging method. The skips correspond to the ray paths of acoustic waves travelling between surface points through the solar interior.

- This project will build on an extensive body of theory developed by the supervisors
- You will examine the sensitivity of the time-distance far-side imaging technique to the size of active regions
- Will to a parameter study of multiple skip theory
- Will work with data which are filtered in the Fourier domain, and only waves that travel long enough to return to the near side from the back side after four and five rebounces are kept.
- Will help understand ghost images in far side imaging

Additional relevant information

It would be expected that the student may spend time in Boulder. Parallel programming and C and Unix coding is part of the skills accumulated during this candidature.

Tachocline

Supervisors

*Prof. Paul Cally (School of Mathematical Sciences, Monash University)
Dr. Mausumi Dikpati (High Altitude Observatory, National Center for Atmospheric Research, Boulder, Colorado)

*Email: paul.cally@monash.edu

Background

The sun rotates about once every 28 days … at the surface … at the equator. The *differential rotation* of the interior has now been mapped using helioseismology, and found to vary greatly with latitude. It also varies somewhat with depth, particularly at the base of the convection zone (r = 0.713 $R_\odot$) where there is a powerful shear layer, the tachocline. There is good reason to believe that the tachocline may be the source of large scale magnetic fields that rise to the surface and form sunspots.

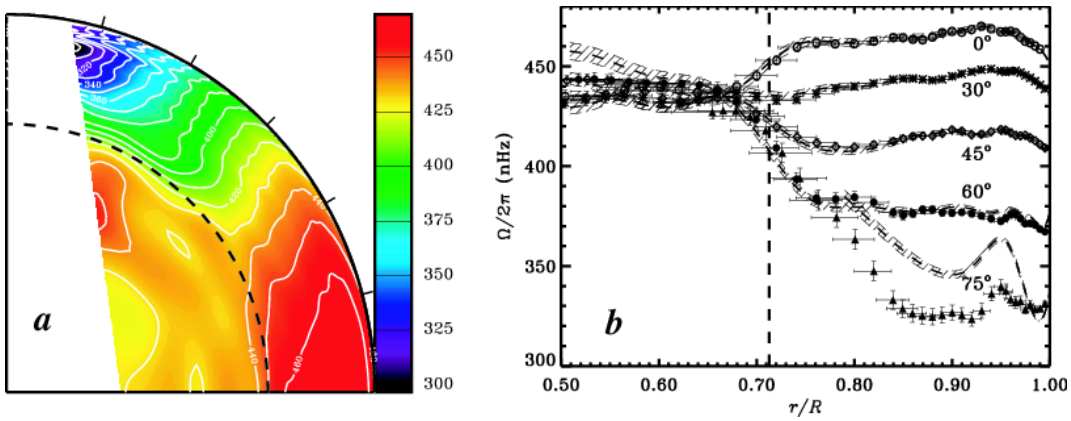


Figure 2 Rotation rates (in nHz) inside the sun. Left: a meridional slice (containing the rotation axes); Right: rotation rate as a function of radius at various latitudes. The dashed curves indicate the base of the convection zone, which lies in the tachocline.

This project will build on an extensive body of theory developed by the supervisors, exploring magneto-shear instabilities that may develop in the tachocline and potentially seed magnetic activity. Linear and nonlinear 2D analyses, "shallow water" theory, Boussinesq 3D, and more extensive 3D magnetohydrodynamic (MHD) simulations will be performed to provide flux to Flux Transport Dynamo models, and for comparison with observed surface activity.

Additional relevant information

Application will be made to one of several suitable HAO/NCAR schemes (Newkirk, Graduate Research Fellow, and visitor, as appropriate) to fund extended visits to the High

Altitude Observatory for collaboration with Mausumi Dikpati. It would be expected that the student may spend up to half their candidature there. Collaborations with Prof Rainer Hollerbach (Leeds) are also likely (3D simulations).

Capturing CO2 with Metal-Organic Frameworks

Supervisors

*Dr Aaron Thornton (CSIRO)
Dr Xavier Mulet (CSIRO)
A/Prof. Matthew Hill (CSIRO and Monash University School of Chemical Engineering)
Prof. Kate Smith-Miles (MAXIMA and the Monash University School of Mathematical Sciences)

*Email: aaron.thornton@csiro.au

Background

MOFs (or Metal-Organic Frameworks) are an advanced material that are extremely ordered, porous, tuneable, and are well known for their host-guest chemistry. Much is known about MOFs and computational studies have shown there are over 100,000 variety of materials that have the potential to be porous systems.

This project will involve the design and production of new MOFs for the purpose of CO_2 capture from direct air. You will be working in a group that specialises in computational studies and the production of MOFs.

The capture efficiency of the MOF is governed by the molecular structure which can be modelled from theoretical ideas. From the molecular-scale to the final product, there are many unknown mechanisms and variables that need to be modelled, understood and optimized.

Additional relevant information

For interested students there is the possibility of a $10,000 top up scholarship associated with this project.

Topics in geological fluid dynamics

Supervisors

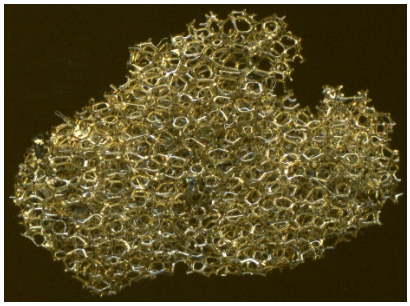
*Dr Anja Slim (School of Mathematical Sciences and School of Earth, Atmosphere and Environment)

*Email: anja.slim@monash.edu

Background

Topic 1: As magma from the mantle rises through the crust, droplets of liquid sulfide can be transported upwards. These droplets have substantially different properties from the host magma: they are about 1.5 times as dense and orders of magnitude less viscous. Some metals such as copper, nickel and platinum group elements become concentrated into these droplets and if the droplets themselves accumulate, then significant ore deposits are formed. Many fluid dynamical questions remain as to the formation of such ores, from the mechanisms of magma-network development to the flow, deposition and redistribution of liquid sulphides within the network. Projects here would combine theoretical modelling with simulations and/or analogue experiments to better understand particular processes. They would involve collaboration with geologists at Monash and at CSIRO in Perth.

Topic 2: When does a volcano erupt explosively and when does it gently effuse? The viscosity of the magma is key. For high viscosity magmas, trapped bubbles cannot escape but expand ever more as the magma rises, forming a magmatic foam that ruptures and erupts explosively. For low viscosity magmas, trapped bubbles can escape and the volcano erupts effusively. This project would develop theoretical and computational models for bubble growth and foam development to better understand explosive eruptions and the range of eruption products such as reticulite (below left), scoria (centre) and pumice (right).



Dynamical Systems of Inertial Particles: A New Kind of Solid-Liquid Separation

Supervisors

*Dr. Guy Metcalfe (School of Mathematical Sciences)
Prof. Murray Rudman (Department of Mechanical and Aerospace Engineering)

*Email: guy.metcalfe@monash.edu

Background

Solid-liquid separation holds a dominant place in the chemicals, minerals, pharmaceutical, food, water and waste processing industries. Around half of capital, operating and energy costs in these industries are consumed in separation processes [1]. As it is imperative for these industries to increase product purity, to reduce waste, to cope with new biotech processes that are relatively dilute and to cope with reduced raw material quality, so is it imperative to foster new solid-liquid separation science. While there are myriad specific solid-liquid separation techniques, they broadly fall into two categories: either particles move through a constrained liquid (sedimentation/flotation), or liquid moves through constrained particles (filtration). However, a third and unexpected category of solid-liquid separation physics has recently been demonstrated [2] whereby particles can spontaneously localize or cluster into small regions of fluid and which, moreover, permits manipulation of particle location according to particle inertia.

This is new physical phenomena, and we have a lot to learn. The student will have every opportunity to break new ground. The student will broaden and deepen our understanding of this phenomenon through theoretical and computational development for wider classes of objects and flows. Current theory is valid for spherical particles, but extension to droplets, cells (deformable objects in general) and anisotropic particles should prove valuable and has no precedent in the literature. Likewise, extending the results to larger and smaller scale flows and to flows at the microfluidic scale will provide further insight into this new phenomenon.

Recommended reading/viewing:

[1] Solid-Liquid Separation (2000) L. Svarovsky, 4th edition, Elsevier Science.
[2] Solid-Liquid Separation by Particle-Flow-Instability (2014) S. Wang, GM, et al Energy & Environmental Science 7(12) 3982—3988, doi:10.1039/C4EE02841D.

Advanced dynamic electrochemistry with Bayesian inference

Supervisors

Prof Alan M Bond and Dr Jie Zhang (School of Chemistry)
Dr Jonathan Keith (School of Mathematical Sciences)

Email: alan.bond@monash.edu
Email: jie.zhang@monash.edu
Email: jonathan.keith@monash.edu

Background

Dynamic electrochemistry (voltammetry) requires the interpretation of potential-current-time relationships obtained at an electrode, and detailed statistically supported comparisons of experimental and theoretical data are almost unknown. At best, and only for a simple electrochemical process, results deduced from a data optimisation (curve fitting) exercise may be provided. Commonly, trial and error estimation of parameters, devoid of any measure of uncertainty are still reported. In this so-called heuristic method of data analysis, the experimenter arbitrarily decides when satisfactory agreement between experimental data and a finally chosen set of simulated data has been achieved in his/her opinion. Continued widespread use of the heuristic methods into the 21st century has arguably limited advances in the level of complexity of problems that could be addressed if automated optimisation methods, grounded in statistical theory and now used routinely across computational science, were to be introduced as a standard practice into reporting experiment- versus theory comparison in the analysis of dynamic electrochemistry.

Aided by the rapid advances in computational power, Bayesian methods coupled with simulation-based Monte-Carlo techniques utilising efficient algorithms such as Gibbs sampling, the Metropolis-Hastings algorithm, and, more recently, Approximate Bayesian Computation, have revolutionised scientists' ability to fit complex mathematical and computational models to experimental data in fields as disparate as astronomy and systems biology. Inspired by these achievements, we will introduce Bayesian inference methods to analyse dynamic electrochemical data, in order to quantify the uncertainty associated with numerous parameters required to describe complex and important problems that abound in the discipline. Crucially, these techniques provide the means not only to provide estimates of key parameters of interest (in dynamic electrochemistry these are typically the kinetic and thermodynamic parameters governing the behaviour of the system under study), but also to quantify the uncertainty associated with those parameters i.e. rather than point estimates, probability distributions of each parameter are returned. In turn, this allows the problem of model selection (i.e. the problem of determining which of two or more competing mathematical models best fits the data) to be addressed in a consistent mathematical framework.

The student employed for this project will be focused on the development of Bayesian inference for data analysis and will also have a chance to work closely with the chemistry students to understand the significance of their projects on a chemical context.

Additional relevant information

The successful candidates will have an opportunity to undertake some of their studies in the University of Oxford, UK, during their PhD candidature.

Quantitative probing of the heterogeneity of electrode surfaces

Supervisors

Dr Jie Zhang and Prof Alan M Bond (School of Chemistry)
Dr Mark Flegg (School of Mathematical Sciences)

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Background

In dynamic electrochemistry, a very powerful analytical chemistry tool, a time dependent potential waveform is employed to a metallic electrode to drive an interfacial electron transfer process. The resulting current provides information about kinetics, thermodynamics and mass transport associated with the heterogeneous electron transfer process. Mercury and amalgam have been common choices of electrode materials for about half century. One of the major advantage of these electromaterials is that their surface is homogeneous and is easily renewable. Consequently, highly reproducible data can be obtained. Moreover, the electrode kinetics in any location of the electrode surface are expected to be the same. Therefore, a simple theory can be used for data analysis to extract quantitative kinetic and thermodynamic information. Unfortunately, mercury has been banned nowadays due to its high toxicity. The commonly used electrode materials, such as Pt, Au and glassy carbon, normally possess considerable heterogeneity. This heterogeneity becomes even more significant with modern carbon based electromaterials, such as boron doped diamond electrodes (due to the non-uniform distribution of boron dopant) and carbon nanotube and graphene (due to the presence of edges/planes, defects and functional groups). When using electrodes made of these materials for electrochemical measurements, it is also probable that the impact of heterogeneity of electrode surfaces will need to be accommodated in comparing different theoretical models with experimental data. This phenomenon is predicted to be much more pronounced at lower mass transport rates applying in ionic liquid voltammetry. To date, the quantitative impact of heterogeneous mass transport has only been considered occasionally, largely due to the introduction of substantial mathematical complexity. To quantitatively take into the effects of the electrode heterogeneity on dynamic electrochemical response, the heterogeneity is often approximated with a highly symmetrical ring-disc type of arrangement so that a three dimensional mass transport problem can be simplified with a two dimensional one as illustrated in Fig. 1a. Then the following partial differential equation that takes into

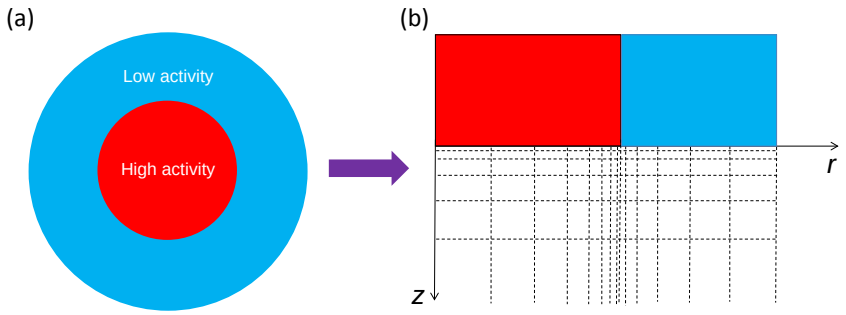

Figure 1. (a) Approximation of surface heterogeneity with a symmetrical ring-disc arrangement for mathematic simplification. (b) Unequal spaced grid in a [*r*, *z*] coordinate.

account the contribution from mass transport and chemical reaction can be solved numerically to obtained spatial (r, z) and time (t) dependent concentration (c) for the calculation of current,

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2}\right) + \text{Chemical Reaction Terms}$$

Due to the presence of heterogeneity (typically of μm size), the current density is expected to be non-uniformed across the electrode surface. An unequal spaced grid in a [r, z] coordinate, illustrated in Fig. 1b, is commonly required to solve the partial differential equations with high accuracy and efficiency. Although the commercial fluid dynamic simulation software package, such as COMSOL Multiphysics®, has the capability to solve the problems of mass transport coupled with chemical reactions, the computation efficiency is inadequate. A more efficient algorithm than the existing ones should be developed to solve the above two-dimensional mass transport equations taking into account the impact of surface heterogeneity.

Additional relevant information

The successful candidates will have an opportunity to undertake some of their studies in the University of Oxford, UK, during their PhD candidature.

Matheuristic Algorithms for Synchromodal Logistics

Supervisors

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Background

Australia's capital cities are becoming increasingly congested. This has many ramifications, including the impacts on container movements. The focus of this project is on finding ways to make transport by rail more efficient to move more of the container movements more efficient, particularly into and out of major ports located in urban areas. This is an industry sponsored project focussing on integer programming optimisation methods and modelling of the intermodal movement of containers. Factors that have to be considered include:

- Ship loading/unloading and possibly temporary storage at the port,
- Train and truck unloading/loading at the port,
- Routing of containers via possibly one or more inland terminals,
- Mode choice between trains and trucks and scheduling of container movements,
- Storage at the inland terminals as well as scheduling of loading and unloading operations.
-

At the strategic level, choices need to be made regarding capital investment decisions relating to railing capacities, truck fleets, equipment for handling containers at the terminals and storage capacities. Operating this transport infrastructure in a synchromodal manner requires adaptively making decisions on timing, mode choice and routing of container movements. Container movements are restricted by release times and due dates, that is time windows between which they must be picked up and delivered. These time windows are typically determined by customers and shipping companies and subject to change. The travel times of trucks are also likely to vary significantly during periods of congestion. Hence the need for an adaptive, synchromodal operating mode.

Additional relevant information

There are two PhD projects available in this area focussing on strategic network design and adaptive logistic operations respectively. As part of the ARC Linkage project there is funding for 2 top-up scholarships and additional conference travel support.

Development of Stocks Network Models

Supervisors

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Background

The advances of big data analysis raise many challenging problems for studying large-scale complex networks. One of the networks is stocks correlation network that explores the connection and relationship between different stocks. Each node of the network stands for a stock. The edge with weight connecting a pair of stocks represents the correlation between these two stocks. The random matrix theory was first applied to study the complicated financial system, analyzed the fluctuations of stocks market. Research results suggested that stock networks satisfy small-world and scale-free properties. Studies also showed that the stocks connecting with a large amount of other stocks have more common economic factor than stocks connecting with less stocks. Through the New York Stock Exchange, a research work verified that the influence posed on all stocks occurs almost simultaneously whether it is from economy or politics.

Among these studies, the Pearson's Correlation coefficient is the main tool to measure the relationship between two nodes. However, it can only measure linear relationship. There are other approaches to measure the relationship. For example, mutual information is a more general way to measure nonlinear relationships and has a wide range of applications. Stocks network based on mutual information or mutual information rate were studied. However, research in this area is still at the early developmental stage.

To build the stocks network, the commonly used algorithms are the Minimum Spanning Tree, Planar Maximum Filter Graph, and Correlation Coefficient Threshold Method [1,2,3]. But a single method could not be able to extract all the economic information from correlation coefficient matrix of a stock portfolio. The topological analysis is useful in the search of economic factors affecting stock prices.

To address these issues, this project will propose new frameworks to develop stock network. We will use the stock price data from the Australian Securities Exchanges (ASX) and Shanghai Stocks Exchange (SSE) will be used to demonstrate the effectiveness of the new approach.

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