QANZIAM MEETING 2019

QANZIAM — The Queensland Branch of ANZIAM

Australian and New Zealand
Industrial and Applied Mathematics Society

Room 204
Building 45 (Mansergh Shaw)
University of Queensland
St Lucia, Brisbane QLD
4 June 2019

QANZIAM MEETING (Tuesday 4th June, 2019)

8.30-9.00	Registration (Room 204, Building 45)	
9.00-9.05	Welcome	
9.05-9.20	CLAUDIO ARANCIBIA-IBARRA*	Spatial patterns in a diffusive Holling–Tanner predator-prey model with weak Allee effect on the prey
9.20-9.35	CHANTELLE BLACHUT*	Detecting fundamental changes to coherent structures in non-autonomous dynamical systems
9.35-9.50	ALEXANDER BROWNING*	A Bayesian sequential learning framework to parametrise a model of melanoma invasion into human skin
9.50-10.05	NICHOLAS BUTTLE*	Computation and analysis of gravity-capillary waves
10.05-10.20	JOSHUA CALCUTT*	Convective transport of capillary loops in the viable skin
10.20-10.35	SOLENE HEGARTY-CREMER*	A cell-based particle method for modelling hyperbolic curvature flows in biological tissue growth
10.35-11.00	Morning tea	
11.00-12.00	**Invited speaker** BRONWYN HAJEK	Analytic solutions for reaction-diffusion equations with applications to calcium fertilisation waves
12.00-12.15	ABBISH KAMALAKKANNAN*	Utilising Generalised Polynomial Chaos to refine the design of an electrode array to measure cardiac conductivities
12.15-12.30	JUSTIN KENNEDY*	Detection of parametric roll resonance using Bayesian Discrete-Frequency model selection
12.30-12.45	MATTHEW KING*	Dissipation in a quartic potential
12.45-1.00	YIFEI LI*	Travelling wave solutions in a negative nonlinear diffusion-reaction model
1.00-2.00	Lunch (Alumni Court)	
2.00-2.15	NATHAN MARCH*	A fast semi-analytical homogenization method for block, locally-isotropic heterogeneous media
2.15-2.30	LIAM MORROW*	A flexible numerical scheme for investigating non-standard Hele-Shaw configurations
2.30-2.45	RYAN MURPHY*	An individual-based mechanical model of cell movement in heterogeneous tissues and its coarse-grained approximation
2.45-3.00	DILAN PATHIRANA*	Possible causes of pre- and post-treatment observations in Coarctation of the Aorta patients
3.00-3.15	NIZHUM RAHMAN*	Travelling wave solutions of a 1D model for collective cell migration in an epithelial layer
3.15-3.30	JESSE SHARP*	Optimal control of acute myeloid leukaemia
3.30-3.45	ANUDEEP SURENDRAN*	Spatial structure arising from chase-escape interactions with crowding
3.45-4.15	Afternoon tea	
4.15-4.30	SEAN VITTADELLO*	Mathematical models of cell proliferation in experiments exhibiting cell-cycle synchronisation
4.30-4.45	DAVID WARNE*	Accelerating Bayesian inference for stochastic models by preconditioning with approximate continuum limit descriptions
4.45-5.00	ANDREW WILKINS	Modelling mosquito gene drives in Africa
5.00-5.30	QANZIAM Meeting	

Student talks asterisked

Abstract of invited talk

Analytic solutions for reaction-diffusion equations with applications to calcium fertilisation waves

Dr Bronwyn Hajek

School of Information Technology and Mathematical Sciences, University of South Australia, Adelaide

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Nonlinear reaction- diffusion equations are used widely to model many different systems and processes, particularly in biology. In this talk, I'll show how the nonclassical symmetry method can be used to find analytic solutions to nonlinear reaction-nonlinear diffusion equations. Provided the nonlinear reaction and nonlinear diffusion terms are related in a certain way, there exists a nonclassical symmetry that gives rise to a transformation that will linearise and separate (in time and space) the reaction-diffusion equation, so that analytic solutions may be constructed. In this talk, I'll describe the application of this technique to solve the equations describing calcium fertilisation waves in both amphibian and mammalian eggs.

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Abstracts of contributed talks in order of presentation

Spatial patterns in a diffusive Holling–Tanner predator-prey model with weak Allee effect on the prey

Claudio Arancibia-Ibarra, Michael Bode, José Flores, Peter van Heijster

In this work, we consider temporal and spatio-temporal Holling–Tanner predator-prey models with Holling type II functional response and weak Allee effect on the prey. We show that the model has at most three equilibrium points in the first quadrant, one is always a saddle point while the other two can be a repeller and/or an attractor. From our results of the temporal model, we identify regions in parameter space in which Turing instabilities in the spatio-temporal model are expected for two of the equilibrium points. Subsequently, we analyse these instabilities. We use simulations to illustrate the behaviour of both the temporal and spatio-temporal model.

Detecting fundamental changes to coherent structures in non-autonomous dynamical systems

Chantelle Blachut, Cecilia González-Tokman

The ability to detect and characterise the dynamic behaviour of coherent structures in a non-autonomous dynamical system can lead to a better understanding of how mass is transported. Here we develop and implement algorithms that detect the merging and separation of coherent structures in a complex system under a time-dependent flow. Coherent structures are regions of phase space that disperse minimally over time even though their location and boundaries might vary. The singular value decomposition (SVD) of a transfer operator induced by a dynamical system provides us with a multi-layered characterisation of that system for a given time interval. Such a decomposition is useful for identifying the regions of phase space that exhibit maximal coherence. Our work considers the SVD of a cocycle of numerically estimated Ulam matrices for a time-dependent dynamical system and investigates the evolution of the relevant singular vectors and singular values over time. Results show this method allows one to retrieve important information regarding the location and time windows of interest within which coherent structures merge and separate, in the presence of an underlying time-dependent (possibly) chaotic flow.

A Bayesian sequential learning framework to parametrise a model of melanoma invasion into human skin

Alexander Browning, Matthew Simpson

We present a novel framework to parameterise a mathematical model of melanoma cell invasion into human skin. Our technique uses a suite of increasingly sophisticated experimental data to sequentially estimate the proliferation rate, diffusivity and a parameter that quantities the invasion of the cells into human skin. Our Bayesian sequential learning approach is simple to implement, computationally efficient and leads to well-defined parameter estimates. In contrast, taking a naive approach that attempts to estimate all parameters from a single set of data from the same experiment fails to produce meaningful results.

Computation and analysis of gravity-capillary waves

Nicholas Buttle, Scott McCue, Timothy Moroney

The waves behind a ship moving with a constant velocity have a very distinct pattern. On this large scale, gravity is the dominant force on the surface. We wish to study smaller scale problems, such that surface tension has a noticeable effect on the surface profile. Using Fourier transforms, we derive analytic solutions to the linearised problem. We then separate the solution into four separate components representing the near-field gravity and near-field capillary, and far-field gravity and far-field capillary waves. We analyse the resulting wake patterns using a time-frequency analysis to extract the different components of the wake. This is comparable to analysing real-world ship wakes using a single, stationary sensor with a ship travelling past.

Convective Transport of Capillary Loops in the Viable Skin

Joshua Calcutt, Yuri Anissimov

Transdermal drug delivery is an attractive form of drug delivery as it has a large area of application, bypasses first-pass metabolism, limits toxicology problems and has easy application. However, in the past, the stratum corneum barrier has limited the number of drugs that could be applied transdermally. The development of transdermal technologies in recent years has minimised the effect of the stratum corneum barrier and thus made the transport of a solute in the viable skin far more critical. However, mathematical modelling in this area of the skin is limited in its applicability and physiological relevance. For this reason, a physiological-based model has been developed to predict the viable skin and dermal concentration in the skin. In this model, the capillary loops in the skin have been explicitly modelled to represent the vascular network present. By modelling the convective nature of these capillary loops, a much more accurate representation of the transient profiles of transdermal drugs has been obtained. The convection of the capillary loops has also significantly changed the steady-state profile as the loops carry the drug to deeper regions of the viable skin.

A cell-based particle method for modelling hyperbolic curvature flows in biological tissue growth

Solene Hegarty-Cremer, Pascal Buenzli, Matthew Simpson

This project adapts the so-called cell-based particle method (CBPM) to simulate the motion of biological tissue boundaries subject to a certain type of geometric control. The cell-based particle method (CBPM) is a hybrid front-tracking method able to handle complex geometries and topological changes easily. The CBPM relies on marker particles on the moving interface as well as an underlying grid. The grid is used to redistribute the marker particles after their evolution, and to search for neighbouring marker particles. This method has been used successfully to evolve PDEs on evolving surfaces using standard finite difference schemes, and is therefore well-suited to be adapted for hyperbolic curvature flows. Hyperbolic curvature flows can describe the deposition of new tissue in porous bioscafolds and in bone pores during bone remodelling. The method is compared to previous owrks in simple tissue geometries and is qualitatively compared to experimental bone infilling data.

Utilising General Polynomial Chaos to Refine the Design of an Electrode Array to Measure Cardiac Conductivities

Abbish Kamalakkannan, Peter Johnston, Barbara Johnston

Cardiac diseases continue to be some of the most prevalent illnesses worldwide due to fundamental gaps in knowledge about the functioning of the heart. Simulation studies, based on mathematical modelling, are increasingly becoming a valuable tool that can be used to explore and hence find treatments for such cardiac diseases. However, such models are reliant on fundamental parameters of the heart - one such being the cardiac conductivities which describe the electrical conduction in the three orthogonal directions in cardiac tissue. To date, a consensus does not exist on these values, with considerable variation in the sets of measured conductivities.

Recent simulation studies have demonstrated that it is possible to retrieve accurate cardiac conductivity values through the use of an electrode array on which cardiac potentials are measured. An inversion technique is further utilised to obtain the cardiac conductivities with the aid of the bidomain model of cardiac tissue. However, the difficulties lie both in making the potential measurements on the electrode array and in interpreting these measurements. This talk looks at implementing a Generalised Polynomial Chaos-based technique to produce a map of sensitivities of output potentials to the input conductivities in a slab model of cardiac tissue. This data can then be utilised to re-design the electrode array to retrieve more accurate cardiac conductivities.

Detection of Parametric Roll Resonance using Bayesian Discrete-Frequency Model Selection

Justin M. Kennedy, Jason J. Ford, Tristan Perez, Francis Valentinis

This paper explores the use of two discrete-frequency models and a probabilistic Bayesian model selection procedure to detect the inception of parametric resonance in ships. We exploit knowledge of the coupling between roll and pitch due to the restoring forces arising from the shape of the hull to propose a single and a double discrete-frequency model. These models are then used within a Bayesian framework to compute the posterior distribution of the frequencies and amplitudes of the two models and this information is used for model selection. The latter is based on the computation of the probability that each one of the models is correct given the data analysed within a past window of samples. The algorithm is tested with data from a scale-model experiment for both regular and irregular sea states. The results indicate the proposed detector is effective in accusing the inception of parametric resonance.

Dissipation in a quartic potential

Matthew King, Owen Jepps

Identifying relaxation to equilibrium, or to non-equilibrium steady states, remains a challenge in contemporary statistical mechanics. A large part of the difficulty has been in finding phase functions that are able to describe fundamentally thermodynamic concepts such as dissipation. One phase function that has been proposed recently is the so-called Dissipation Function, which is closely related to the divergence of the dynamical equations of motion (which is traditionally used to describe entropy production rates in non-equilibrium statistical physics). There remains ongoing work to achieve a deeper understanding of how one can interpret results involving the Dissipation Function in the context of relaxation processes. We have studied relaxation to equilibrium in simple micro-canonical systems of interacting particles trapped in harmonic or quartic wells, to help shed further light on the interpretation of the Dissipation Function as it relates to equilibration processes. To our knowledge, this is the first application of the DF to a micro-canonical system.

Travelling wave solutions in a negative nonlinear diffusion-reaction model

Yifei Li, Petrus van Heijster, Matthew Simpson

Nonlinear diffusion-reaction equations naturally arise as continuum limits of lattice-based discrete models considering birth, death and movement events of agents that are isolated or grouped. The mathematical analysis of these equations is in its infancy, especially for nonlinear diffusivity functions that can become negative.

We use a geometric approach and prove the existence of smooth travelling wave solutions of a nonlinear diffusion-reaction equation with logistic kinetics and a convex nonlinear diffusivity function which changes sign twice in our domain of interest. We further determine the minimum wave speed, c^*, and investigate its relation to the spectral stability of the travelling wave solutions.

A fast semi-analytical homogenization method for block, locally-isotropic heterogeneous media

Nathan March, Elliot Carr, Ian Turner

Direct numerical simulation of flow through heterogeneous media can be difficult due to the computational cost of resolving fine-scale heterogeneities. One method to overcome this difficulty is to coarse-grain the model by decomposing the domain into a number of smaller sub-domains and homogenizing the heterogeneous medium within each sub-domain. In the resulting coarse-grained model, the fine-scale diffusivity on each sub-domain is replaced by an effective diffusivity, calculated from the solution of an appropriate boundary value problem over the sub-domain. However, in simulations in which the heterogeneous sub-domain geometries evolve over time, the effective diffusivities need to be repeatedly recomputed and may bottleneck a simulation. In this presentation, I will present a new semi-analytical method for solving the boundary value problem and computing the effective diffusivity for block locally-isotropic heterogeneous media. I will compare the new method to a standard finite volume method and show that the equivalent accuracy can be achieved in less computational time for several standard test cases. I will also demonstrate how the new method can be used to homogenize complex heterogeneous geometries represented by a grid of blocks.

A flexible numerical scheme for investigating non-standard Hele-Shaw configurations

Liam Morrow, Scott McCue, Timothy Moroney

A commonly used tool for studying interfacial instabilities is the Hele-Shaw cell, which is an experimental apparatus made of two parallel plates separated by a narrow gap. When an inviscid fluid is injected into a Hele-Shaw which is otherwise filled with a viscous fluid, the interface generally is unstable and forms distinct patterns. In recent years, there has been interest in determining how manipulating the geometry of the Hele-Shaw can influence and control the development of these patterns. Such manipulations include lifting the plates as the bubble is injected, tapering the plates, or rotating the Hele-Shaw cell. While numerical methods for solving the standard Hele-Shaw problem are well-established, often they cannot be extended to incorporate these changes in geometry. Here we present a scheme based on the level set method capable of solving a general model of the Hele-Shaw cell, and show that numerical simulations compare well with experimental results.

An individual-based mechanical model of cell movement in heterogeneous tissues and its coarse-grained approximation

Ryan Murphy, Pascal Buenzli, Ruth Baker, Matthew Simpson

Mechanical heterogeneity in biological tissues, in particular stiffness, can be used to distinguish between healthy and diseased states. However, it is often difficult to explore relationships between cellular-level properties and tissue-level outcomes when biological experiments are performed at a single scale only. To overcome this difficulty we develop a multi-scale mathematical model which provides a clear framework to explore these connections across biological scales. Starting with an individual-based mechanical model of cell movement, we subsequently derive a novel coarse-grained system of partial differential equations governing the evolution of the cell density due to heterogeneous cellular properties. We demonstrate that solutions of the individual-based model converge to numerical solutions of the coarse-grained model, for both slowly-varying-in-space and rapidly-varying-in-space cellular properties. We discuss applications of the model, such as determining relative cellular-level properties and an interpretation of data from a breast cancer detection experiment.

Possible Causes of Pre- and Post-treatment Observations in Coarctation of the Aorta Patients

Dilan Pathirana, Barbara Johnston, Peter Johnston

Coarctation of the Aorta (CoA) is a poorly diagnosed, serious congenital heart disease with several treatment options available. Reviews of the disease conclude that additional clinical data are required in order to compare the different treatments in terms of their long-term health outcomes.

Although there are several treatments for CoA, the available data suggest that patients treated differently often experience similar mid- and long-term negative health outcomes, including increased incidence of late hypertension and a decreased life expectancy, compared to healthy people.

Due to the lack of clinical data, we ran simulations involving a one-dimensional mathematical model of blood flow and a network model of the 56 largest arteries in the human body, to study whether coarctations, abnormalities associated with CoA, or the resection & end-to-end anastomosis or stent treatments, produce altered blood flow properties that may contribute to negative long-term health effects in patients.

We find that increased arterial stiffness in the upper body produces blood flow properties that are observed in patients, pre- and post-treatment. These results suggest reasons for why early diagnosis of CoA is difficult, and why treating the coarctation alone does not resolve all of the health issues that are observed in CoA patients pre-treatment.

Travelling wave solutions of a 1D model for collective cell migration in an epithelial layer

Nizhum Rahman, Dietmar Oelz

For a 1D model for collective cell migration in epithelial layers we find various travelling wave solutions which correspond to polarisation and depolarisation waves associated to either colliding or diverging layers of cells. We discuss the parameter regimes which determine the stability of these solutions and their relevance in model wound assays.

Optimal control of acute myeloid leukaemia

Jesse Sharp, Kevin Burrage, Matthew Simpson

Acute myeloid leukaemia (AML) is a blood cancer affecting the haematopoietic stem cells of the myeloid cell line. AML is routinely treated with chemotherapy, incurring significant health and financial cost, so it is of great interest to develop optimal chemotherapy treatment strategies. In this talk, we incorporate an immune response into a stem cell model of AML, since we find that previous models lacking an immune response are inappropriate for predicting optimal control strategies. Using optimal control theory, we can produce continuous controls and bang-bang controls, corresponding to a range of objectives and parameter choices. We provide a practical discussion of the implementation of optimal control to the AML model. In particular, we describe and explore factors that impact numerical convergence.

Spatial structure arising from chase-escape interactions with crowding

Anudeep Surendran, Michael Plank, Matthew Simpson

Movement of individuals, mediated by localised interactions, plays a key role in numerous processes including cellular biophysics and ecology. In this work, we propose an individual based model (IBM) of multispecies motility that accounts for various intraspecies and interspecies interactions in a community that is composed of an arbitrary number of distinct species. This framework allows us to explore how individual-level directional interactions scale up to influence spatial structure at the macroscale. To focus exclusively on the role of motility and directional bias in determining spatial structure, we consider conservative communities where the number of individuals in each species remains constant. We derive a mathematically tractable deterministic approximation of the IBM using an approach based on describing the dynamics of the spatial moments. An important objective of this study is to use the general IBM and spatial moment dynamics frameworks to investigate the impact of interactions in a stereotypical community consisting of two distinct species. We explore how different features of interactions including interaction strength, spatial extent of interaction, and relative density of species influence the formation of the macroscale spatial patterns.

Mathematical models of cell proliferation in experiments exhibiting cell-cycle synchronisation

Sean Vittadello, Scott McCue, Matthew Simpson

A population of cells is synchronised when the cells are in the same cell-cycle phase. In cell proliferation experiments, it is often desirable to have the cells randomly distributed throughout the cell cycle, rather than synchronised. Here we present new cell proliferation experiments which exhibit cell synchronisation, despite following standard experimental procedures to produce asynchronous cell populations. The synchronised cells produce oscillations in the subpopulations of cells corresponding to the phases of the cell cycle. In order to identify these subpopulations, we utilise fluorescent ubiquitination-based cell cycle indicator, or FUCCI, which allows the visualisation of the G1, eS and S/G2/M cell-cycle phases of individual cells. We utilise multi-stage mathematical models of cell proliferation to describe the oscillatory nature of the cell subpopulations when cells are synchronised.

Accelerating Bayesian inference for stochastic models by preconditioning with approximate continuum limit descriptions

David Warne, Matthew Simpson

Ecological and biological sciences rely on the characterisation of populations of interacting individuals. Random walks are standard in modelling the stochastic nature of individual movement, growth and death. Due to the computationally burdensome task of stochastic simulation, it is routine to employ mean-field assumptions to derive approximate continuum limit descriptions of these kinds of stochastic models. Bayesian parameter inference is especially prohibitive for random walks since expensive likelihood-free methods are required. Conversely, the approximate continuum limit description yields a closed-form likelihood. However, for parameter regimes where the mean-field approximation is inaccurate, statistical inferences are biased. We propose that, despite this bias, the approximate continuum limit may still be exploited to accelerate Bayesian inference for expensive random walk models. Specifically, we extend sequential Monte Carlo sampling algorithms for approximate Bayesian computation. Our methods utilise samples from the continuum limit posterior as a precondtioner to inform efficient sampling from the target posterior for the random walk model. The resulting methods are demostrated to be effective at significantly reducing the number of expensive stochastic simulations while maintaining accuracy in parameter and uncertainty estimates.

Modelling mosquito gene drives in Africa

Andrew Wilkins

Genetically altering mosquitoes offers the potential to eliminate mosquito-borne diseases such as malaria. CSIRO is part of a large world-wide effort to study the impacts and efficacy of such alterations. I will present a simple and fun ODE model that describes the interactions of two sub-species of mosquito, one of which is an proposed target for a genetic alteration. I will also present some results from a numerical model of spatial spread.