NSW-ACT ANZIAM Meeting

University of Newcastle, City Campus

(Corner of Hunter St & Auckland St, Newcastle NSW 2300)

19-20 November 2018





Meeting Timetable

·	
12.20 - 12.50	$Registration - Room \ X202$
12.50-13.00	Opening welcome
Chair	Chris Lustri
13.00-13.35	Elena Levchenko – Statistical mechanical analysis of diffusion
	kinetics in liquid alloys
13.35-13.55	Benjamin Maldon [*] – Modelling dye-sensitized solar cells by
	nonlinear diffusion
13.55-14.15	Carl Omerod [*] – Opening a 'window' on diffusion for
	CRDD development
14.15-14.35	Balaje Kayanaraman [*] – Mathematical models for ice shelf
	vibrations
14.35-15.05	Afternoon tea
Chair	Bishnu Lamichhane
15.05-15.40	Linda Stals – Multilevel methods for the thin-plate spline
	saddle point problem
15.40-16.00	Yihong Du – The Fisher-KPP equation over simple graphs:
	Varied persistence states in river networks
16.00 -16.20	Xiaoping Lu – A PDE approach for weather derivative pricing
16.20-16.40	Dong Yan [*] – Pricing options with stochastic volatility
	and transaction costs
16.40-17.00	Tom Futcher [*] – An analytical formulation to the optimal
	exit price of stock loans
17.00-17.30	NSW ANZIAM branch meeting

Monday 19 November 2018

Chair	Mike Meylan
9.00-9.35	Deborah Cromer – Using Mathematical Modelling to understand
	HIV reactivation
9.35-9.55	Fillipe Georgiou [*] – Continuum model for phagocytosis based on
	cell-cell adhesion and prey-predator relationship
9.55-10.15	David Khoury – Host mechanisms of control during acute
	malaria infection
10.15-10.35	Mark Nelson – No Jab, no pay
10.35-10.55	Michael Lydeamore – Estimating epidemiological quantities for skin
	sores in remote Australian communities using interval-censored data
10.55-11.25	Morning tea
Chair	Mark Nelson
11.25-12.00	Marianito Rodrigo – Revisiting the time-fractional diffusion-wave
	equation
12.00-12.20	Mike Meylan – Flexural gravity wave blocking and Hawking radiation
12.20-12.40	Chris Lustri – Generalised solitary waves in discrete integrable systems
12.40-13.00	Marcia Pinheiro – S-convex functions, examples: incursions
	into real analysis
13.00-13.10	Conclusion
13.10-14.30	Lunch

Tuesday 20 November 2018

*Presentation by PhD student

[†]Conference Dinner will be at Scratchleys on the Wharf http://www.scratchleys.com.au/ 200 Wharf Road, Newcastle Phone: 02 4929 1111 Note: Meals are included in the registration fee, but please pay for your own drinks.



Organising Committee

Prof Natalie Thamwattana (University of Newcastle) A/Prof Mark Nelson (University of Wollongong) Dr Christopher Lustri (Macquarie University) Dr David Allingham (University of Newcastle) Mrs Juliane Turner (University of Newcastle)

Abstracts

Using Mathematical Modelling to understand HIV Reactivation <u>Deborah Cromer</u>

The Kirby Institute, University of New South Wales

Current HIV therapies are able to suppress the virus to undetectable levels, and allow people living with HIV to lead relatively symptom-free lives. However as soon as therapy is stopped the virus "rebounds" and leads to increased HIV associated morbidity. This rebound is due to a latent reservoir of HIV infected cells that are not killed by current therapies and can reactivate months or years after becoming infected.

One of the main focuses of HIV research today concerns allowing people living with HIV to experience prolonged periods where they do not need to remain on treatment. Allowing such a "treatment holiday" requires an understanding of the time it would take for virus to appear when treatment is stopped, the factors influencing this "viral rebound" and the population level effects of such increases in virus.

We have used mathematical models combined with various clinical and experimental datasets to estimate key parameters of viral rebound as well as to determine clinical factors that may be predictive of faster or slower rebound. Additionally, we have combined these quantitative estimates with a model of HIV remission and reactivation to estimate the impact of various new modes of therapy that may be able to reduce the size of the latent reservoir.

Our work shows that while therapies designed to reduce the size of the latent reservoir present a promising avenue of research, prior to widespread implementation of such strategies, both the drivers and consequences of viral reactivation from latency must be adequately considered.

The Fisher-KPP equation over simple graphs: Varied persistence states in river networks Yihong Du

University of New England

I'll report a recent work with my collaborators, on the growth and spread of a new species in a river network with two or three branches via the Fisher-KPP advection-diffusion equation, over some simple graphs with every edge a half infinite line. We obtain a rather complete description of the long-time dynamical behavior for every case under consideration, which can be loosely described by a trichotomy, including two different kinds of persistence states as parameters vary. The phenomenon of "persistence below carrying capacity" revealed here appears new, which does not occur in related models of the existing literature where the river network is represented by graphs with finite-lengthed edges, or the river network is simplified to a single infinite line.

An analytical formulation to the optimal exit price of stock loans <u>Tom Futcher*</u> University of Wollongong

An approximation to the optimal exit price for stock loans is obtained where it is assumed the dividend is reinvested immediately after being paid. The PDE system is first converted to a dimensionless system and then converted to the Laplace space. The methodology present in Zhu (2006) is used which involves the pseudo steady-state approximation which arises in the Stefan problem. Once the appropriate expression has been determined in the Laplace space, an appropriate contour integral is constructed to obtain an expression for the optimal exit price of a stock loan. The variables are converted back to their dimensional quantities when calculating the numerical results to demonstrate the behaviour of the optimal exit price.

Continuum model for phagocytosis based on cell-cell adhesion and prey-predator relationship

Filipe Georgiou^{*} University of Newcastle

Phagocytosis is defined as ingestion of large ($\geq 0.5\mu$ m) particles, such as unwanted cells, debris or particulate matter, into plasma membrane-derived vacuoles called phagosomes. This process is accomplished via the use of receptors on the cells surface that recognize and bind to the prey particles. Phagocytosis plays an important role in immune systems through the destruction of pathogens and the inhibiting of cancerous cells. We combine a cell-cell adhesion modelling technique with classic predator-prey modelling to generate a new model for phagocytosis which can relate the interaction between cells in both space and time. Using this model we create numerical simulations in both one and two dimensions, we compare the two dimensional simulation with a video of bacteria phagocytized by neutrophil cell. We also look at dispersion relations for both homogeneous and non-homogeneous steady states for one-dimensional model to look at the range of parameters that will lead to phagocytosis.

Seismometer measuements on the Ross Ice Shelf have confirmed the presence of ocean wave induced vibrations by various components of ocean waves - from the longer tsunamiinfragravity waves to the shorter ocean-swell waves. Mathematical models have been developed assuming that the incident wavelengths are much greater than the shelf thickness and the ocean depth. These models make use of the Euler-Bernoulli beam theory for the ice coupled with the linear shallow water equations for the fluid motion. However, the shallow water assumptions are generally valid in the infragravity regime but not valid in the open ocean for ocean-swell waves as the wavelengths are comparable to the ocean depth. To model the fluid motion in such cases, a more complicated finite depth model is required.

In this talk, we discuss the mathematical model where we use the Euler-Bernoulli beam theory for the ice and the finite depth model for the fluid. The model is then solved using the eigenfunction matching method and the solution is then compared with the solution of the shallow water model. We show that the latter is generally not valid for incident wave time periods less than 50 s. Further, we relax the thin-shelf assumption and employ the full linear elasticity equations for the ice and observe that the thin-shelf assumption breaks down for lower values of time period. We then plot the stress distribution along the thickness of the ice which can then be used predict the collapse of the ice-shelf.

Host mechanisms of control during acute malaria infection

David Khoury, Rosemary Aogo, Deborah Cromer, Ashraful Haque, Miles P. Davenport The Kirby Institute, University of New South Wales

Malaria is responsible for almost half a million deaths each year. Overly intense inflammation by the host immune system in response to infection has long been implicated in severe disease due to malaria. However, obviously host immune responses to acute malaria infection are also known to be critical for survival. Surprisingly little is understood about the impact of host immune responses during acute infection on controlling parasite growth. For example, one hypothesis of the role of many different host responses during acute infection is that they all assist in driving more removal of parasites by the spleen (an organ that has a major role in filtering the blood). Host removal of parasites (or parasite clearance) has long been suspected as a major mechanism of host control of infection. However, no explicit quantification of host clearance of parasites or how much host removal is improved during acute infection have been made. Here we combined modelling of within host parasite replication with unique experimental data to measure host removal of parasites. Surprisingly, rather than finding that individual malaria infected red blood cells are removed more rapidly by the host during acute infection, we find that individual infected cells persist in circulation for longer. Using an age-structed first order PDE model of parasite development we identified that this extended parasite persistence in circulation is likely due to a delayed parasite development (parasites taking longer to complete their life-cycle). Further analysis has revealed that various manipulations of the host response can induce and abrogate delayed development.

Statistical Mechanical Analysis of Diffusion Kinetics in Liquid Alloys

Elena V. Levchenko

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This talk will feature recent advances which have been achieved in the course of theoretical understanding of interrelation between single-particle and collective diffusion in binary melts by my team [1,2]. These theoretical insights are in particular of significant importance for engineering the crystalline microstructure in the framework of phase field modelling of the complex branched morphologies exhibited by dendrites during solidification from melt.

The presented mathematical analysis of diffusion kinetics in a binary melt has been carried out in the framework of the Mori-Zwanzig formalism of statistical mechanics. As a result, an analytical expression, relating the Onsager coefficient for mass transport, L_{cc} , to the two single-particle (self-diffusion) coefficients, D_1 and D_2 , of species in a binary melt, has been derived as

$$\tilde{L}_{cc} = S(c_2 D_1 + c_1 D_2), \qquad S = S_0 \left(1 + \frac{W_{12}}{k_B T} \right), \qquad S_0 = \frac{m^2 D_1 D_2}{m^2 D_1 D_2 + c_1 c_2 (m_1 D_1 - m_2 D_2)^2}.$$

We have shown that this expression is a superior alternative to the well-known Darken equation. The derived expression naturally accounts for manifestation of microscopic (dynamic) cross-correlation effects in the kinetics of collective diffusion and can be presented in a form which explicitly incorporates the correction factor *S* into the Darken equation. Furthermore, it has been demonstrated that the correction factor *S* can be decomposed into the product of two other factors. The first factor $S_0 \leq 1$ is expressed in terms of the ratio of the self-diffusion diffusion coefficients D_1/D_2 , the ratio of the atomic masses m_1/m_2 , and the alloy composition c_1 (or c_2 , $c_1 + c_2 = 1$), while the second factor is related to a collective energy generation-dissipation effect (term W_{12}/k_BT) due to the correlations between fluctuations of the interdiffusion flux and the force caused by the difference in the average random accelerations of atoms of different species.

We have argued that for binary mixing melts exhibiting chemical ordering (such as Ni-Al and Ni-Zr melts) the correction factor should typically be $S < S_0$ ($W_{12} < 0$), while for binary melts where precursors of liquid–liquid demixing are important (such as Cu-Ag melts) the correction factor should be $S > S_0$ ($W_{12} > 0$). Furthermore, we have identified that in thermal equilibrium the correction factor should be within the range $0 \le S \le 2S_0$, which is constrained by the energy of thermal fluctuations ($|W_{12}| \le k_B T$). Moreover, the results of our analysis can be used to suggest a concept of a binary liquid random alloy for which $W_{12} = 0$, so that the correction factor $S = S_0$. Lastly, we have demonstrated an application of our analysis for interpretation of recent experimental studies and our molecular dynamics simulations [1-3] of diffusion kinetics in binary melts.

Acknowledgements

I would like to acknowledge the support of the Australian Research Council (Grant ARC DP170101812) and CARMA.

References

- [1] E.V. Levchenko, A.V. Evteev, Insight into interrelation between single-particle and collective diffusion in binary melts, *Physica A: Statistical Mechanics and its Applications* **490** (2018) 1446-1453.
- [2] A. Kromik, E.V. Levchenko, C. Massobrio, A.V. Evteev, Diffusion in Ni-Zr melts: Insights from statistical mechanics and atomistic modelling, *Advanced Theory and Simulations* (2018) 1800109-14.
- [3] E.V. Levchenko, T. Ahmed, A.V. Evteev, Composition dependence of diffusion and thermotransport in Ni-Al melts: A step towards molecular dynamics assisted databases, *Acta Materialia* 136 (2017) 74-89.

A PDE approach for weather derivative pricing <u>Xiaoping Lu</u> University of Wollongong

We propose a PDE (partial differential equation) based approach to price weather derivatives with the market price of risk (MPR) extracted from the utility indifference valuation. The PDE system is solved numerically using a one-sided finite difference scheme. The solution procedure is validated through numerical experiments for the utility indifference future prices, and then applied to price more complicated weather derivatives such as options.

Generalised Solitary Waves in Discrete Integrable Systems Christopher Lustri Macquarie University

Generalized solitary waves are nonlinear travelling wave with a central core that exhibits classical solitary wave behaviour, as well as non-decaying oscillations that continue away from the core indefinitely in one or both directions, and have amplitude that is exponentially small in some asymptotic parameter. This behaviour is typically associated with singular perturbations of some system, where the unperturbed system has classical solitary wave solutions.

I will show that discretizations of the KdV equation produce generalized solitary wave solutions in the continuum limit, even if the equation being discretized is not singularly perturbed, nor does it have some natural small parameter. I will then discuss the effect of discretization on relevant bifurcation parameters, by comparing the behaviour of the continuous and discretized versions of a singularly-perturbed fifth-order KdV equations.

Estimating epidemiological quantities for skin sores in remote Australian communities using interval-censored data <u>Michael Lydeamore</u>

The Kirby Institute, University of New South Wales

Prevalence of impetigo (skin sores) remains high in remote Australian Aboriginal communities, Fiji, and other areas of socio-economic disadvantage. Skin sore infections, driven primarily in these settings by Group A Streptococcus (GAS) contribute substantially to the disease burden in these areas. Despite this, estimates for the force of infection, infectious period and basic reproductive ratio — all necessary for the construction of dynamic transmission models — have not been obtained. By utilising three datasets each containing longitudinal infection information on individuals, we estimate each of these epidemiologically important parameters. With an eye to future study design, we also quantify the optimal sampling intervals for obtaining information about these parameters. We verify the estimation method through a simulation estimation study, and test each dataset to ensure suitability to the estimation method. We find that the force of infection differs by population prevalence, and the infectious period is estimated to be between 12 and 20 days. We also find that optimal sampling interval depends on setting, with an optimal sampling interval between 9 and 11 days in a high prevalence setting, and 21 and 27 days for a lower prevalence setting. These estimates unlock future model-based investigations on the transmission dynamics of GAS and skin sores.

Modelling Dye-Sensitized Solar Cells by Nonlinear Diffusion Benjamin Maldon^{*} University of Newcastle

Dye-Sensitized Solar Cells (DSSCs) maintain high research interest, owing to their potential as a viable solution to the renewable energy problem.

While ample nanomaterials have been suggested to improve their efficiency, mathematical modelling and analysis remains noticeably sparse. The dominant model in this area remains the electron diffusion equation, which has been extended to include time-dependence and nonlinear characteristics since its introduction 24 years ago.

In this talk, we analyse this diffusion equation by Lie Symmetry and Homotopy methods and compare results to standard finite difference numerical solutions to obtain the characteristic traits of a DSSC.

Flexural Gravity Wave blocking and Hawking Radiation <u>Mike Meylan</u> University of Newcastle

Flexural gravity waves occur when water waves propagate under an elastic cover. They are used to model waves under a frozen fluid or to model waves in very large floating structures, such as a floating airport. In a recent series of papers with colleagues, I have investigated flexural gravity wave propagation under various conditions. We have focused on some of the very strange behaviours that occurs, such as wave blocking, negative energy waves and even under exceptional circumstances the existence of Hawking radiation. The latter phenomena, while originally proposed for Black Holes, is a phenomenon of classical wave physics.

> No Jab, no pay <u>Mark Nelson</u>, Matthew Giffard University of Wollongong

Before vaccination campaigns in the 1960s and 1970s disease such as diphtheria, tetanus, and whooping cough were responsible for killing thousands of children in Australia. Wide-spread vaccination programs have almost eliminated the death of children from these disease in Australia.

Opponents to vaccination have existed for as long as vaccination itself. The anti-vaccination movement received a major boost in 1998 with the publication of a, now discredited, study in the Lancet which claimed that the mumps, measles and rubella (MMR) vaccine was related to autism. The publication of this study has lead to an increase in the number of opponents to vaccination.

What is the possible effect of the anti-vaccination movement upon the spread of contagious disease?

To answer this question we combine the standard SIR model with vaccination for the spread of a contagious disease with a, slightly modified, SIR model for the spread of the

anti-vaccination contagion. This leads to a system of nine differential equations. We use this model to investigate how the spread of the anti-vaccination contagion within a town increases the number of infections of an infectious disease (assumed to be measles) over a twenty-year time frame.

This is joint work with Matthew Giffard, a second-year undergraduate student at the University of Wollongong.

Opening a 'window' on diffusion for CRDD development <u>Carl Ormerod*</u> University of Wollongong

See last page.

S-convex Functions, Examples: Incursions into Real Analysis Marcia Pinheiro

Generators for the phenomenon S-convexity: they provide functions that fit the new version of the definition.

Revisiting the time-fractional diffusion-wave equation

Marianito Rodrigo University of Wollongong

We consider a nonhomogeneous time-fractional diffusion-wave equation, i.e. when the time derivatives of the classical diffusion and wave equations are replaced by fractional derivatives. We give a new formulation of the solutions to the associated initial value problems in terms of a new special function. The Green's function solution of the heat equation and the d'Alembert solution of the wave equation are recovered as special cases. An overview of the fractional calculus will be provided.

Multilevel Methods For The Thin-Plate Spline Saddle Point Problem Linda Stals Australian National University

Data fitting is an integral part of a number of applications including data mining, 3D reconstruction of geometric models, image warping and medical image analysis. A commonly used method for fitting functions to data is the thin-plate spline method. This method is popular because it is not sensitive to noise in the data.

We have developed a discrete thin-plate spline approximation technique that uses local basis functions. With this approach the system of equations is sparse and its size depends only on the number of points in the discrete grid, not the number of data points. Nevertheless the resulting system is a saddle point problem that can be ill-conditioned for certain choices of parameters. In this talk I will present a combination of multilevel based preconditioners that works well for a wide choice of parameters.

Pricing options with stochastic volatility and transaction costs $\frac{\text{Dong Yan}^*}{\text{University of Wollongong}}$

Our study is concerned with pricing of European-type option with stochastic volatility and transaction costs. When taking the transaction costs into consideration, the option price is no longer unique for the holder and writer of the option due to the market incompleteness. We derive two non-linear PDEs for the holder and the writer of the option, respectively, under the Heston model. The PDEs are solved numerically by Euler explicit method. As it expected our numerical results show that the higher the transaction costs, the lower the option holding price and conversely, the higher the option writing price.

Opening a 'window' on diffusion for CRDD development.

There is increasing interest in the use of diatom species and their porous silica components in *controlled-release delivery devices* (CRDDs) for drugs, nutraceuticals, fertilizers and other applications [1]. Diatoms are extremely successful and a virtually unlimited renewable resource – about 25% of global organic carbon is attributed directly to their photosynthesis [1]. Over 100,000 known species show myriad, fine-structure geometries with pore sizes as small as 20nm. Their success is crucially dependent on efficient transport via micro- and nano-scale ports in their tough, yet elastic, silica *frustules*. Further, their large surface area $(18.5 \pm 0.8 \text{ m}^2/\text{g})$ allows for a plethora of existing chemical functional modification techniques [2].

Biotemplating, the use of natural systems as templates, offers many advantages over synthetic production. Existing Porous SiO_2 drug delivery systems are more expensive, time-consuming, polluting and have poorer pharmacokinetics. New designs using diatomite nano-particles may enable safer reservoir-style delivery devices, which generally show bi-phasic release with an initial burst mode followed by near zero-order, protracted controlled release profiles that cannot be matched by matrix devices. This is especially valid for lipophilic drugs, which constitute an increasingly large portion of modern pharmacy [1, 3].



Figure 1: (A) The marine diatom *Thalassiosira weissflogii* is abundant, scales rapidly, has a small genome and a thoroughly investigated silicic acid transport system (scale bar = 40 μ m). (B) Arrow highlights girdle bands alongside diatom frustule (scale bar = 5 μ m). (C) External view of valve face with arrows highlighting both marginal and central fultoportulae (scale bar = 3 μ m). (D) Zoomed-in view of central fultoportulae (scale bar = 1 μ m). *With permission* [2]

Very few (...er, none) of the existing models used in device development recognize surface heterogeneity, despite the obvious radial patterning [3, 4, 5]. This effectively means they ignore the porthole structure by assuming a uniform surface in every direction. A mixed-boundary solution opens 'windows' in the walls allowing more accurate calculation without resorting to brute force methods like CFD.

A numerical scheme is developed for comparison/calibration and then used to examine the effect of porthole size and position on the time for 90% mass transfer.

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- 1 Foreshore Promenade & Park Newcastle Railway Station, Bus Terminus, Customs House, Lumberyard, Foreshore Promenade & Park, Newcastle's Famous Tram stop
- 2 Hunter Street Mall Shopping & dining, overhead bridge access to Ferry Terminal, Queens Wharf Tower & harbour-side restaurants
- 3 Darby Street Funky inner-city eat street also great for shopping & art lovers
- 4 Newcastle Museum Open Tuesdays to Sundays, 10am-5pm, and seven days a week during school holidays. Free entry
- 5 Maritime Centre & Visitor Information Centre, antiques, cafés & restaurants
- 6 Honeysuckle Drive Government/corporate offices, residential apartments, retail, restaurants and cafés

- 7 Newcastle Marina Newcastle Cruising Yacht Club, Newcastle Fisherman's Co-op & shared cycle/pedestrian path
- 8 8 9 Newcastle West Curious & second-hand bargains
- 10 Islington Alternate walk to Beaumont St via Islington's antique & bric-a-brac stores
- 11 Hamilton Inner-city residential area
- 12 & 13 Beaumont Street Cosmopolitan street with many boutiques & sidewalk cafés
- 14 Tudor Street Closest stop for walking to Newcastle Jockey Club
- 15 Auto Alley A wide range of dealerships in close proximity & Sacred Heart Cathedral
- 16 **TAFE** Hunter Institute of Technology

- 17 Sports & Shopping Precinct No. 1 & 2 Sportsgrounds, netball courts & Marketown Shopping Centre
- 18 Supermarkets and Fast Food Outlets Panthers Newcastle, McDonalds & Marketown Shopping Centre
- 19 Civic Cultural Precinct Civic Park, City Hall, Newcastle Art Gallery, Conservatorium of Music, Newcastle Library & Lovett Gallery, Cooks Hill Gallery & Darby Street. Art deco Civic Theatre & Wheeler Place a unique event destination
- 20 King Street Stores Boutique shopping & cinema
- 21 Cathedral Closest stop for walk to iconic Christ Church Cathedral, the Obelisk. King Edward Park & lookouts
- 22 Newcastle East Precinct Heritage buildings & significant sites, beachside cafés & unique restaurants walk through to Newcastle Beach

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