CTAC 2018

The Priority Research Centre for Computer-Assisted Research in Mathematics and Applications (CARMA) of the University of Newcastle

Newcastle City Hall, Newcastle, New South Wales

27–30 November 2018

Editors: Bishnu Lamichhane, David Allingham and Mike Meylan

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Mathematics of Computation and Optimisation

The CSIRO-ANZIAM Student Support Scheme

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Keynote and Public Speakers

- **Prof. Robert Eymard (Université Paris-Est Marne-la-Vallée)**
- **Prof. Mary Myerscough (University of Sydney)**
- **Dr Matthias Kabel (Fraunhofer Institute for Industrial Mathematics)**
- **Prof. Andreas Prohl (University of Tuebingen, Germany)**
- **Prof. Steve Roberts (Australian National University)**
- **Dr Vera Roshchina (University of NSW)**
- **Prof. Ian Sloan (University of NSW)**
- **Prof. Ian Turner (Queensland University of Technology)** ***(Public speaker)***

Welcome

The 19th Biennial Computational Techniques and Applications Conference (CTAC2018) is hosted by the Priority Research Centre for Computer-Assisted Research Mathematics and its Applications (CARMA) of the University of Newcastle at the Newcastle City Hall.

CTAC is organised by the special interest group in computational techniques and applications of ANZIAM, the Australian and New Zealand Industrial and Applied Mathematics Division of the Australian Mathematical Society. The meeting will provide an interactive forum for researchers interested in the development and use of computational methods applied to engineering, scientific and other problems. The CTAC meetings have been taking place biennially since 1981, the most recent being held in 2016 at Monash University Caulfield Campus.

A refereed proceedings will be published after the conference in the Electronic Supplement of the ANZIAM Journal. This will be subject to the usual rigorous ANZIAM J. refereeing process.

We will have two student prizes, one sponsored by Modelling and Simulation Society of Australia and New Zealand (MODSIM) and the other by Mathematics of Computation and Optimisation (MoCaO). Student talks are denoted in the conference program and list of abstracts by an asterisk.

We hope you enjoy the conference.

Information

Conference venue

The conference is hosted at Newcastle City Hall. All keynote talks including the public talk will be held in Hunter Room. Contributed talks will be held in Hunter room, Newcastle Room 1 and Mulubinba Room, whereas morning and afternoon tea and lunch will be catered in Banquet Room. The Computational Mathematics Group meeting will take place in Newcastle Room 1 at 5pm on Thursday before the public lecture. We will have a light refreshment in Hunter Room before the public lecture. The layout of the Newcastle City Hall is attached at the end of the booklet.

Presentations

All plenary talks are 50 minutes long, plus 5 minutes for questions. All contributed talks are 25 minutes long, plus 5 minutes for questions, discussion and changeover. The session chair will give you a signal when you have 5 minutes remaining. Please do not exceed your time.

Each lecture theatre is equipped with a laptop computer running Windows, with mouse, keyboard, USB ports, and Internet connection. There is also a fixed data projector and a projection screen. We strongly encourage you to bring your talk in the form of a *PDF document*. You may bring it on a USB storage device or email it to the organisers. Please make sure that your talk is copied onto the laptop computer before the session of your talk.

If you require access to other software packages or other audio-visual equipments please talk to the organisers well in advance to see whether it can be arranged.

It is possible to connect your personal laptop to the data projector, but we prefer that you avoid this option due to the tight conference schedule. If you insist, please contact the session chair to test the connection well before your presentation.

Internet access

Wifi details will be as follows:

Network: CTACConf

Password: Newcastle27 (case sensitive)

Social events

We will have a welcome reception with drinks and canapés in Hunter Room from 5–7 pm on Tuesday, 27th of November. The conference dinner will be held at 7:00 pm on Wednesday, 28th of November at Noah's On The Beach, which is around 20 minutes walking distance from the Newcastle City Hall. The address of *Noah's On The Beach* is 29 Zaara Street, Newcastle NSW 2300. A map of the hotel *Noah's On The Beach* is included at the end of this booklet.

Travel to and from the airport

- Sydney Airport to Newcastle For those arriving at Sydney Airport we recommend taking the train most of the way to Newcastle (the train line into Newcastle has been truncated and you will need to transfer to a bus or other alternative at Hamilton Station). For information and trip planning, please visit transportnsw.info.

You should take the T2 Airport Line from Domestic/International Airport Station to Central Station and then the Central Coast & Newcastle Line Hamilton Station. From Hamilton Station you must transfer to a bus into the city.

Alternatively, there is the Hunter Connection airport shuttle, which you will need to book in advance.

- Newcastle Airport to Newcastle For those arriving at the Newcastle Airport we recommend taking a taxi to Newcastle. The taxi rank is adjacent to the arrivals area of the terminal. Newcastle Taxis can be contacted directly, free-of-charge, on the dedicated taxi phone located in the arrivals end of the terminal.

  Alternatively, you can catch the 130 or 131 bus from the Newcastle Airport to the Newcastle Station. From Newcastle Station it is an easy walk to the recommended hotels. For more information and/or to plan your exact trip times see the Sydney Trains or the Port Stephens Coaches timetables.

Local Transportation in Newcastle

Newcastle Taxis: bookings can be made online or by calling 133 300 within Australia. For public transport options, please visit transportnsw.info.

Dining

There are a number of restaurants near the conference venue.

Programme

Tuesday 27th November	
5.00pm-7.00pm	**Registration and Welcome Reception in Hunter Room**

Wednesday 28th November			
8.20-8.50am	**Registration in Hunter Room**		
8.50-9.00am	**Welcome address, Bishnu Lamichhane, President of CMG**		
9.00-10:00am	Ian Sloan (p.16) *Computational probing of the Cosmic Microwave Backgound maps*		
	Newcastle Room Chairs: Frances Kuo	Mulubinba Room Linda Stals	Hunter Room Vera Roshchina
10.00-10.30am	Yuancheng Zhou* (p.42) *The application of sparse grid quadrature in solving stochastic optimization problems*	Hideaki Nagasaka* (p.37) *Use of block Arnoldi method for the efficient numerical solution of nonlinear eigenvalue problems*	Layth Awin* (p.23) *Numerical Simulation for Entrainment in Forced Turbulent Fountains*
10.30-11:00am	Fanzi Meng* (p.36) *Multi-fidelity sparse girds for uncertainty quantification*	Mohamed Al-Sultani* (p.22) *Block monotone iterative methods for solving coupled systems of nonlinear elliptic problems*	Oliver Krzysik* (p.30) *Parallel time integration of PDEs with multigrid methods*
Morning tea			
Plenary chair	**Thanh Tran**		
11.30-12.30am	Andreas Prohl (p.17) *Simulation of nonlinear SPDEs: Convergence Analysis and Adaptivity*		
Lunch			
Plenary chair	**David Jenkins**		
1.30-2.30pm	Matthias Kabel (p.17) *Poroelastic behavior of rocks using Digital Rock Physics*		
	Newcastle Room Chairs: Jerome Droniou	Mulubinba Room Feng-Nan Hwang	Hunter Room Vesa Kaarnioja
2.30-3.00pm	Abhishek Bhardwaj* (p.23) *Numerical view of Polynomial Systems*	Hanz Martin Cheng* (p.25) *A combined GDM–ELLAM–MMOC (GEM) scheme for advection dominated PDEs*	Vesa Kaarnioja (p.29) *Stochastic collocation for electrical impedance tomography with applications to stroke imaging*
3.00-3.30pm	Kim Ngan Le (p.31) *Convergent numerical methods for nonlinear porous media equations*	Nathan March* (p.34) *Finite volume schemes for multilayer diffusion*	Riya Aggarwal* (p.22) *Finite Element Approach to Bragg Edge Neutron Transmission Strain Tomography*
Afternoon tea			

Wednesday 28th November			
	Newcastle Room Chairs: Mike Meylan	Mulubinba Room Mary Myerscough	Hunter Room Elliot Carr
4:00-4.30pm	Jordan Pitt* (p.39) *A Finite Element-Volume Method for the Serre Equations*	Benjamin Maldon* (p.33) *Numerical Solutions to the Nonlinear Electron Diffusion Equation in Dye-Sensitized Solar Cells*	Neil Dizon* (p.26) *Optimization in the Construction of Symmetric and Cardinal Wavelets on the Line*
4.30-5.00pm	Balaje Kalyanaraman* (p.30) *Mathematical Models for Ice Shelf Vibrations*	Gopikrishnan Chirappurathu Remesan* (p.25) *Numerical solution of the two-phase tumour growth model with moving boundary*	Lishan Fang* (p.27) *Error indication and adaptive refinement of the discrete thin-plate spline smoother*
7.00-10.00pm	**Conference Dinner at Noah's On The Beach**		

Thursday 29th November			
Plenary chair	Mike Meylan		
9.00-10.00am	Mary Myerscough (p.16) *Mathematical models for the immunology of atherosclerotic plaques*		
	Newcastle Room Chairs: Stephen Roberts	Mulubinba Room Quoc Thong Le Gia	Hunter Room Shev MacNamara
10.00-10.30am	Kaichung Wong* (p.42) *Numerical Investigation and Modelling of the Venous Injection of Sclerosant Foam*	Joe Peach* (p.38) *A spectral method for the stochastic Stokes equations on the sphere*	Stacey Osbrough* (p.38) *The Effects of Model Climate Bias on ENSO Variability and Ensemble Prediction*
10.30-11.00am	Fillipe Georgiou* (p.27) *An adaptive numerical scheme for a partial integro-differential equation*	Xifu Sun* (p.41) *Parameter Estimation for Computationally Expensive "Black Box" Models in the Bayesian Framework*	Julius F. Rabago* (p.39) *A novel shape optimization formulation of the exterior Bernoulli free boundary problem*
Morning tea			
Plenary chair	Jerome Droniou		
11.30-12.30pm	Robert Eymard (p.16) *Approximation of linear convection problems using the Gradient Discretisation Method*		
Lunch			
Plenary chair	Linda Stals		
1.30-2.30pm	Vera Roshchina (p.18) *Projection methods: convergence and counterexamples*		
	Newcastle Room Chairs: Torsten Linß	Mulubinba Room Andreas Prohl	Hunter Room Robert Eymard
2.30-3.00pm	Tania Prvan (p.39) *Generalised smoothing splines in a stochastic setting*	Brendan Harding (p.28) *The computation of inertial lift force on a spherical particle suspended in flow through microfluidic ducts*	Jerome Droniou (p.26) *A high-order scheme for the Brinkman model*
3.00-3.30pm	Linda Stals (p.40) *Multilevel Solvers for The Thin-Plate Spline Saddle Point*	Shev MacNamara (p.33) *Comparison of Precipitation and Temperature Trends between Coastal and Inland New South Wales*	Markus Hegland (p.28) *Numerical methods for computing the GCD of univariate polynomials using floating point arithmetic*
3.40-4.00	Students prizes presentation in Hunter Room		
Afternoon tea			

Thursday 29th November	
5.00-5.30pm	**CMG meeting (Newcastle Room 1)**
Public lecture chair	**Markus Hegland**
6:00-7:00pm	Ian Turner (p.19) *Computational Modelling for Industry*

Friday 30th November			
Plenary chair	**Markus Hegland**		
9.00-10.00am	Stephen Roberts (p.18) *Sparse-Grid-Based Uncertainty Quantification Applied to Tsunami Run-up and Inundation*		
	Newcastle Room Chairs: Brendan Harding	Mulubinba Room Tania Prvan	Hunter Room Thanh Tran
10.00-10.30am	Elliot Carr (p.24) *Novel calculation of response times for groundwater flow*	Björn Rüffer (p.40) *Non-convex feasibility, Douglas–Rachford, and Lyapunov functions*	Torsten Linß (p.32) *Maximum-norm a posteriori error bounds for parabolic problems*
10.30-11.00am	Geordie McBain (p.35) *Three ways to compute multiport inertance*	Vivien Challis (p.24) *Optimising a family of anisotropic microstructures: computational approach and applications*	Matej Medla (p.35) *Finite volume method for the Geodetic boundary value problem*
Morning tea			
	Newcastle Room Chairs: Brendan Harding	Mulubinba Room Tania Prvan	Hunter Room Thanh Tran
11.30-12:0pm	Feng-Nan Hwang (p.29) *A full-space quasi Lagrange-Newton-Krylov algorithm for 3D multi-stage launch-vehicle trajectory optimization problems*	Mike Meylan (p.36) *The forced vibration of a floating elastic plate*	Simon Watt (p.41) *Competitive combustion reactions in two dimensions*
12.00-12.30pm	Tim Moroney (p.37) *Three dimensional free-surface flow over arbitrary bottom topography*	Elena Levchenko (p.32) *Onsager Coefficient for Collective Diffusion in Binary Melts*	
Lunch and Closing			

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Computational probing of the Cosmic Microwave Backgound maps

Ian Sloan (University of New South Wales)

i.sloan@unsw.edu.au

According to cosmological theory, the cosmic microwave background (CMB) should be to a good approximation a realisation of a Gaussian random field. In this project, joint with Robert Womersley, Thong Le Gia and Yu Guang Wang, we develop a computational tool to probe the CMB temperature maps published by the Planck collaboration. We show that some of the maps, as judged from their Fourier coefficients, depart very significantly from random fields. In the case of the "SEVEM" map we show that the field can be modelled as a random field plus a localised needlet-like structure situated at the galactic centre, with the non-random part being large enough to affect significantly the angular power spectrum.

Mathematical models for the immunology of atherosclerotic plaques

Mary Myerscough (University of Sydney)

mary.myerscough@sydney.edu.au

The formation of atherosclerotic plaques depends on many factors; blood flow, tissue perfusion, cellular emigration, lipid oxidization and cytokine signals, for example.

Computational models, particularly for blood flow and blood vessel morphology, have been important in researching several aspects of this multifactorial pathology. However, key immunological events that occur inside the artery wall as a plaque forms and grows have, until recently, not been well-explored by computational models, even though there is significant scope for improving our understanding of plaque growth and pathology by using mathematical models in this way.

In this talk I will present a suite of models for the behaviour of macrophages and other immune cells, for the fate of cholesterol that enters the plaque and for the movement of smooth muscle cells and the generation of collagen caps that protect plaques from rupture. These models range from simple sets of ODES to integro-partial differential equations, but all require computational solution.

Approximation of linear convection problems using the Gradient Discretisation Method

Robert Eymard (Université Paris-Est Marne-la-Vallée)

Robert.Eymard@u-pem.fr

The gradient discretisation method is a generic framework which encompasses a large number of classical and recent methods for the approximation of elliptic and parabolic problems. We show in this talk how this framework applies to different problems including a linear convection term. We discuss different approaches for the approximation of this term.

Poroelastic behavior of rocks using Digital Rock Physics

Matthias Kabel (Fraunhofer Institute for Industrial Mathematics)

matthias.kabel@itwm.fraunhofer.de

Digital rock physics (DRP) is an image-based workflow that allows estimation of physical rock properties by performing numerical simulations of pore-scale physics (e.g., elasticity, Navier-Stokes) on 3D scans of rock samples. Traditionally, most DRP is done regarding the flow of oil and water but in this talk we will concentrate on mechanical properties taking into account fluid filled pores.

In the first part of our talk we will explain necessary extensions of FFT-based homogenization techniques for the simulation of fluid filled rocks. In the second part, we will demonstrate that the constitutive relations based on the Biot-Gassmann theory are in excellent agreement with our numerical results. The numerical simulation can potentially lead to an improved analysis of the spatial distribution of large stresses induced due to loading of grains.

Simulation of nonlinear SPDEs: Convergence Analysis and Adaptivity

Andreas Prohl (University of Tuebingen, Germany)

prohl@na.uni-tuebingen.de

The stochastic Navier-Stokes equation, or the stochastic version of the harmonic map flow to the 2D sphere are examples for nonlinear SPDEs which only possess weak martingale solutions. In the first talk of my talk, I identify requirements for a discretization of a 'quite general' nonlinear SPDE to construct a weak martingale solution for vanishing discretization parameters.

In the second part, I discuss adaptive concepts to automatically refine space-time meshes via the distance of empirical laws of related iterates: these concepts are applied to e.g. resolve steep gradients inside interfaces in convection dominated SPDEs, or to resolve blow-up dynamics in the case of the stochastic version of the harmonic map flow to the 2D sphere.

These results base upon joint works with M. Ondrejat (Prague), N. Walkington (Pittsburgh), and C. Schellnegger (Tübingen).

Sparse-Grid-Based Uncertainty Quantification Applied to Tsunami Run-up and Inundation

Stephen Roberts (Australian National University)

stephen.roberts@anu.edu.au

Given a numerical simulation, the objective of uncertainty quantification is to provide an output distribution for a quantity of interest given a distribution of uncertain input parameters. However exploring this output distribution using for instance a Monte Carlo strategy requires a high number of numerical simulations, which can make the problem impracticable within a given computational budget.

A well-known approach to reduce the number of required simulations is to construct a surrogate, which — based on a set of training simulations — can provide an inexpensive approximation of the simulation output for any parameter configuration. To further reduce the total cost of the simulations, we can introduce alternative sampling strategies such as sparse grid sampling which can lead to a substantial cost reduction in the construction of a surrogate.

An additional strategy is to augment a reasonably small number of high-resolution training simulations with many cheap low-resolution simulations. This technique can lead to orders of magnitude increase in efficiency in the construction of surrogate models with reasonably high (8-15) dimensional input parameter spaces.

In this talk I will present some methods based around sparse grid approximation for producing efficient surrogate models and demonstrate these methods applied to quantifying the uncertainty in the height and extent of tsunami inundation which has application in evacuation planning.

Projection methods: convergence and counterexamples

Vera Roshchina (University of New South Wales)

v.roshchina@unsw.edu.au

The history of projection methods goes back to von Neumann and his method of alternating projections for finding a point in the intersection of two linear subspaces. These days the method of alternating projections and its various modifications, such as the Douglas-Rachford algorithm, are successfully used to solve challenging feasibility and optimisation problems.

The rate of convergence of projection methods depends on the structure of the sets that comprise the feasibility problem, and also on their position relative to each other. I will survey a selection of classical results, focusing on the impact of error bounds and facial structure of the convex sets on the convergence of projection methods. I will also introduce some recent findings and counterexamples.

Computational Modelling for Industry

Ian Turner (QUT)

ian.turner@qut.edu.au

The QUT porous media modelling group has developed a number of fruitful collabo- rations with industry partners over the last 20 years where large-scale computations

were utilised to investigate and optimise operations. In this lecture I will reflect on the rich experience of working with industry ? from commercial research to work integrated learning for final year students. A pleasing outcome is the impact our research has had on industry practices. A selection of our past modelling projects will be reviewed, including:

1. Forecasting the value of a southern pine plantation.
2. Drying of lignocellulosic materials.
3. Groundwater modelling.

I will also provide a brief survey of the computational solution strategies employed for the models.

This is CTAC public lecture and will be held on Thursday, 29th of November in the Hunter Room at 6:00 pm

Brief Biography: Ian Turner is a professor of computational mathematics in the School of Mathematical Sciences at the Queensland University of Technology. His main research interests are in the fields of computational mathematics and numerical analysis, where he has over thirty years experience in solving systems of coupled, nonlinear partial differential equations that govern flow in porous media. He has published over 250 research articles in a wide cross section of journals spanning science and engineering, and his multidisciplinary research demonstrates a strong interaction with industry. He is also a former Head of School of Mathematical Sciences at QUT. Recently, Professor Turner was named in the 2015, 2016 Thomson Reuters and 2017 Clarivate Analytics Web of Science list of Highly Cited Researchers.

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Finite Element Approach to Bragg Edge Neutron Transmission Strain Tomography

Riya Aggarwal * (University of Newcastle)

Riya.Aggarwal@uon.edu.au

Collaborators: Mike Meylan, Bishnu Lamichhane and Chris Wensrich

Neutron Transmission methods have recently shown promising results in terms of tomographic reconstruction of strain tensor fields within samples. This technique involves reconstruction from sets of Bragg-edge transmission strain images as measured by pixelated time-of-flight neutron detectors at pulsed neutron sources. As opposed to conventional Radon based CT, this revolves around the inversion of the Longitudinal Ray Transform (LRT) which has known issues surrounding uniqueness. In this work, reconstruction is approached via a least squares approach constrained by equilibrium formulated through the finite element method. An example of this approach is provided for a 2D plane-stress situation.

Block monotone iterative methods for solving coupled systems of nonlinear elliptic problems

Mohamed Al-Sultani * (Massey University)

M.Al-Sultani@massey.ac.nz

This talk deals with numerical methods for solving coupled system of nonlinear elliptic problems. We utilize block monotone iterative methods based on the Jacobi and Gauss–Seidel methods to solve a nonlinear system of difference equations which approximate the coupled system of nonlinear elliptic problems, where the reaction functions of these considered systems are either quasimonotone nondecreasing or quasimonotone nonincreasing. Based on the method of upper and lower solutions, two monotone upper and lower sequences of solutions are constructed, where the monotone property ensures the theorem on existence-uniqueness of solutions to the nonlinear discrete system. Construction of initial upper and lower solutions is given. A convergent analysis of the monotone sequences generated by the block Jacobi and the block Gauss-Seidel methods is presented. Numerical experiments illustrate the theoretical results.

Numerical Simulation for Entrainment in Forced Turbulent Fountains

Layth Awin** (The University of Sydney)

lawi8820@uni.sydney.edu.au

Collaborators: Steven Armfield, Nicholas Williamson, Wenxian Lin and Michael Kirkpatrick

Fountains occur when a dense fluid is projected upwards into a less dense fluid. They are widely found in nature and industrial applications such as volcanic eruptions and air conditioning systems. In turbulent fountains, fluid entrainment plays a key role to control the properties of the fountain such as penetration height and width. The control parameters of fountains are typically two non-dimensional numbers, the Froude and Reynolds numbers, where the former characterises the fountain flow as weak or forced while latter characterises the flow as laminar or turbulent. In this study, a computational fluid dynamic technique is applied to investigate the entrainment and general structure of forced turbulent fountains. Simulations for a three-dimensional fountain flow in a rectangular domain are obtained using a nondimensional form of the Navier-Stokes equations. The flow is simulated by solving the governing equations using a finite-volume approach with standard second order discritsations for all spatial terms other than advection, where the ULTRA-QUICK scheme is used. Time integration uses second-order Adams-Bashforth and Crank-Nicolson for the advective and viscous terms respectively with the pressure-correction approach used to enforce continuity and obtain pressure. The numerical simulations were conducted on switched computer clusters to obtain the fully developed flow for a range of Reynolds number, $2000 \leq Re \leq 3500$, and Froude number, $5 \leq Fr \leq 24$. The results show that the properties of fountains are relatively insensitive to the Reynolds number, while they have a linear relation with the Froude number for the cases considered in this study. The entrainment coefficient between the fountain flow and ambient is obtained as well as linear regression scales for height and width in terms of the Froude number.

Numerical view of Polynomial Systems

Abhishek Bhardwaj** (Australian National University)

Abhishek.Bhardwaj@anu.edu.au

Polynomial systems have been widely studied in the areas of Algebraic Geometry. However, research on finding common roots of polynomial systems has only recently begun. In this talk we explore some of the challenges of handling polynomial systems over floating point numbers. We consider also a non-symbolic approach to generating a Groebner Basis, as well as modifications to the Buchberger algorithm for special systems.

Novel calculation of response times for groundwater flow

Elliot Carr (Queensland University of Technology)

elliot.carr@qut.edu.au

Collaborators: Matthew Simpson

When perturbed by a transient response such as a brief rainfall event on the ground surface, an aquifer system will eventually transition to a new equilibrium/steady state. The time required to transition between steady states is often referred to as the response time and is important in many practical situations. A simple way to calculate the response time is to advance the solution of the transient groundwater flow model in time and calculate the time until the difference between the transient and steady-state solutions is below a small specified tolerance. This approach, however, can be computationally expensive as the accuracy of the approach is governed by the size of the time step. In this talk, I will present an alternative method for accurately and efficiently calculating response times for a specific groundwater flow model, the linearised one-dimensional Dupuit-Forcheimer model of saturated flow. The new method expresses the response time in terms of a simple formula involving the temporal moments of an appropriate function representing the transition to steady-state. Attractively, the new approach does not require the solution of the transient groundwater flow model. Numerical results are validated against an existing laboratory-scale data set describing flow in a homogeneous system and a synthetic data set describing flow in a heterogeneous system.

Optimising a family of anisotropic microstructures: computational approach and applications

Vivien Challis (The Unversity of Queensland)

vchallis@maths.uq.edu.au

Collaborators: Andrew Cramer, Tony Roberts

Microstructural optimisation is a computationally expensive engineering design problem where the goal is to find a microstructure that optimises specific physical properties of the resulting material - physical properties such as stiffness or permeability. We are currently interested in optimising multiparametric families of microstructures that encompass a range of material properties. This magnifies the computational expense because the number of microstructural optimisations to perform is large. I'll talk about our computational approach to this problem and show recent results that have significant potential for use in both multiscale structural optimisation and functionally graded materials.

A combined GDM–ELLAM–MMOC (GEM) scheme for advection dominated PDEs

Hanz Martin Cheng * (Monash University)

hanz.cheng@monash.edu

Collaborators: Jerome Droniou and Kim-Ngan Le

We propose a combination of the Eulerian Lagrangian Localised Adjoint Method (ELLAM) and the Modified Method of Characteristics (MMOC) for time-dependent advection-dominated PDEs. The combined scheme, so-called GEM scheme, takes advantages of both ELLAM scheme (mass conservation) and MMOC scheme (easier computations), while at the same time avoids their disadvantages (respectively, harder tracking around the injection regions, and loss of mass).

We present a precise analysis of mass conservation properties for these three schemes and numerical results illustrating the advantages of the GEM scheme. A convergence result of the MMOC scheme, motivated by our previous work on the convergence of ELLAM schemes, is provided, which can be extended to obtain the convergence of GEM scheme.

Numerical solution of the two-phase tumour growth model with moving boundary

Gopikrishnan Chirappurathu Remesan * (Monash University,)

gopikrishnan.chirappurathuremesan@monash.edu

In this work, a novel method has been proposed to tackle the computational difficulties involved while solving the one-dimensional two-phase tumour growth model with a time-dependent boundary. The method consists in defining an equivalent problem in a fixed domain without using any change of variable transformation. The mass and momentum conservation applied to the model variables – volume fraction, pressure, and velocity of tumour cells and extracellular material; and nutrient concentration – gives a coupled system of non-linear advection equation (hyperbolic), generalised stationary Stokes equation (elliptic) and non-linear diffusion equation (parabolic) with suitable conditions on the time-evolving boundary governed by an ordinary differential equation. The standard method for solving this model using hybrid finite volume-finite element schemes require updating of the boundary at each time step. The updated domain needs to be re-meshed further satisfying the Courant-Freidrich-Levy condition to ensure the stability of the finite volume scheme. Extension of the advection equation to a fixed domain, of which every tumour domain up to a fixed time is a subset, overcomes these computational issues. The time-dependent boundary is retrieved, as the hyper-surface at which the solution to the advection equation develops a shock. The other equations do not require an extension, hence are solved in the domain enclosed by this retrieved boundary.

The evolution of the moving boundary is embedded correctly in the extended model as the shock curve and thereby proves the equivalence of the two formulations. A comparison between the results from the implementation and previously available literature shows excellent agreement. This technique can be adapted easily from the one-dimensional case to higher dimensions, and the boundary since being recovered as the shock curve enables us to work with tumours with more realistic shapes.

Optimization in the Construction of Symmetric and Cardinal Wavelets on the Line

Neil Dizon* (The University of Newcastle)

neilkristofer.dizon@uon.edu.au

Collaborators: Jeffrey Hogan, Joseph Lakey

Ingrid Daubechies' construction of compactly supported smooth orthogonal wavelets on the line having multiresolution structure, coupled with other desirable properties, relied heavily on techniques of complex analysis, many of which are unavailable in the higher-dimensional setting. Alternatively, Franklin, Hogan, and Tam developed techniques which have been successful in producing Daubechies' wavelets, among others, from uniform samples of the so-called quadrature filters associated with the multiresolution structure. In this talk, we present an alternative construction of compactly supported smooth orthogonal wavelets by considering samples of the scaling functions and associated wavelets as variables. This allows for the construction of scaling functions and wavelets with optimal cardinality and symmetry properties.

A high-order scheme for the Brinkman model

Jerome Droniou (Monash University)

jerome.droniou@monash.edu

Collaborators: Lorenzo Botti, Daniele Di Pietro

The Brinkman model is an intermediate model between a Darcy flow (in porous media) and a Stokes flow (free flow). It is described by two parameters, the viscosity and the ratio permeability/viscosity, and gives back a Darcy or Stokes flow when these parameters reach certain limits. The model's unknowns are the velocity and pressure of the fluid.

We will present a novel discretisation method of the Brinkman model, based on a hybrid approximation of the velocity and a discontinuous approximation of the pressure. The unknowns are therefore vector-valued polynomials on the faces in the cells for the velocity, and scalar-valued polynomials in the cells for the pressure. The method hinges on higher order reconstructions of the velocity in the cells, which yield optimal rates of convergence. The established error estimates are robust in all limits, from Darcy to Stokes throughout the whole range of intermediate regimes. Numerical results corroborate the theoretical estimates.

Error indication and adaptive refinement of the discrete thin-plate spline smoother

Lishan Fang * (The Australian National University)

Lishan.Fang@anu.edu.au

The thin-plate spline is a technique for interpolating and smoothing surface over scattered data in many dimensions. It is a type of polyharmonic splines that appears in various applications, including image processing and correspondence recovery. It has some favourable properties like being insensitive to noise in data. One major limitation of the thin-plate spline is that the resulting system of equation is dense and the size depends on the number of data points, which is impractical for large datasets.

A discrete thin-plate spline smoother has been developed to approximate thin-plate spline with local basis functions. Its resulting system of equations is sparse and the size depends only on the number of nodes in finite element grid instead of the number of data points. However, a solution with high accuracy will still require a fine grid and a large system of equations. Adaptive refinement of discretisation grids was developed to adapt the precision of the solution within sensitive regions (e.g. peaks, boundaries, singularities, etc.), which can be determined by error indicators. In this talk, I will present some error indicators for the discrete thin-plate spline smoother and compare their performance for different problems.

An adaptive numerical scheme for a partial integro-differential equation

Fillipe Georgiou * (University of Newcastle)

fillipe.georgiou@uon.edu.au

Collaborators: B. Lamichhane and N. Thamwattana

One method of modelling cell-cell adhesion gives rise to a partial integro-differential equation. While non-adaptive techniques work in the numerical modelling of such an equation there are many opportunities for optimisation. The studied partial integro-differential equation has a tendency to produce aggregations leaving large regions where both the function value and derivative are equal to 0 leading to a higher resolution than needed and lower than desired resolution where the aggregations form. In order to overcome this we develop an adaptive scheme in both space and time using a modified form of ODE45 and finite volume methods to more efficiently simulate the studied partial integro-differential equation. We first use our numerical scheme to simulate the problem presented in the original paper and compare results to determine if our numerical scheme works, we then use it to simulate a new and novel situation.

The computation of inertial lift force on a spherical particle suspended in flow through microfluidic ducts

Brendan Harding (The University of Adelaide)

brendan.harding@adelaide.edu.au

Inertial lift force is a second order effect causing particles to deviate from the streamlines of (laminar) fluid flow. Particle trajectories can be calculated via direct numerical simulation, using a Navier-Stokes model of the fluid flow, but this is expensive and not particularly informative. In this talk I describe an approach for estimating the inertial lift force which involves decomposing the problem into a sequence of Stokes equations. This can then be used to locate stable equilibria onto which particles migrate. Further, with a little more work, particle trajectories can be estimated efficiently and a wealth of information on the sensitivity to many of the input parameters can be obtained. I also discuss some aspects of using the open source FEniCS platform to carry out the bulk of the computations.

Numerical methods for computing the GCD of univariate polynomials using floating point arithmetic

Markus Hegland (The Australian National University)

markus.hegland@anu.edu.au

Euclid's algorithm provides a well-known and often used tool to determine the greatest common divisor (GCD) of polynomials with rational coefficients. Unfortunately, when used with floating point arithmetic, the computed GCD is often a constant function even when the exact GCD is a higher degree polynomial. Reasons for this are rounding errors pervasive in floating point computations and errors in the input data. It turns out that the underlying division algorithm (as well as Euclid's algorithm) can be recast as a matrix factorisation and rank determination problem. It can be shown that the LU factorisation which forms the base of Euclid's method exists. However, partial pivoting or rank-revealing QR factorisation methods avoid large rounding errors which may occur for standard LU. Combining this with a thresholding method provides a robust approach for the computation of approximate GCDs. While we will only consider univariate polynomials here, similar stable numerical algebra techniques are even more relevant for multivariate polynomials. While many of these techniques have been studied for dense polynomials which have nonzero coefficients for most monomial basis functions, we will also discuss how to utilise techniques of sparse linear algebra to efficiently compute the GCD of sparse polynomials for which most of the monomial coefficients are zero. This approach uses a symbolic factorisation stage in which the matrix of the problem is computed or assembled. This illustrates the point that computing the GCD requires the computation of the underlying matrix in addition to the solution of the rank determination problem.

A full-space quasi Lagrange-Newton-Krylov algorithm for 3D multi-stage launch-vehicle trajectory optimization problems

Feng-Nan Hwang (National Central University, Taiwan)

hwangf@math.ncu.edu.tw

Collaborators: Hsuan-Hao Wang, Feng-Tai Hwang

The objectives of this work are to apply and study the full-space quasi Lagrange-Newton-Krylov (FQLNK) algorithm for solving trajectory optimization problems arising from aerospace industrial applications. As its name suggests, we first convert the constrained optimization problem into an unconstrained one by introducing the Lagrangian parameters. The next step is to find the optimal candidate solution by solving the Karush-Kuhn-Tucker (KKT) condition with the Newton-Krylov method. To reduce the computational cost of constructing the KKT system, we employ the Broyden-Fletcher-Goldfarb-Shanno (BFGS) formula to build an approximation of the (1,1) subblock of the KKT matrix, which is the most expensive part of the overall computation. The BFGS-based FQLNK algorithm exhibits a superior speedup compared to some of the alternatives, including finite differences and automatic differentiation. We demonstrate our FQLNK algorithm to be a practical approach for designing a 3D optimal trajectory of the multi-stage launch vehicle in space missions.

Stochastic collocation for electrical impedance tomography with applications to stroke imaging

Vesa Kaarnioja (University of New South Wales)

v.kaarnioja@unsw.edu.au

Electrical impedance tomography (EIT) is an imaging modality designed to reconstruct the interior conductivity of an object based on voltage and current measurements on the object's boundary. One of the major benefits of EIT in medical use is that it does not subject patients to radiation. In addition, the affordability and mobility of an EIT device make it an interesting addition to conventional radiation-based imaging devices in hospitals.

Recently, EIT has been investigated as a promising method to diagnose stroke patients in a fast, efficient, and safe manner. In this talk, we explore a parametric model for the cross section of a human head using a Karhunen-Lo?ve type expansion which is used to model uncertainties in the head shape. This results in a high-dimensional EIT forward problem incorporating uncertain model parameters and it is solved by using stochastic collocation based on sparse grids. The collocated forward solution can be used to effectively solve the inverse problem of recovering the interior conductivity and geometry of a human head based on electrode measurements. The effectiveness of this approach is assessed in numerical simulations involving real-life human head geometries with simulated stroke symptoms.

Mathematical Models for Ice Shelf Vibrations

Balaje Kalyanaraman* (University of Newcastle)

Balaje.Kalyanaraman@uon.edu.au

Seismometer measuerments on the Ross Ice Shelf have confirmed the presence of ocean wave induced vibrations by various components of ocean waves - from the longer tsunami-infragravity 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

Parallel time integration of PDEs with multigrid methods

Oliver Krzysik* (Monash University)

oliver.krzysik@monash.edu

Collaborators: Hans De Sterck, Scott MacLachlan, Stephanie Friedhoff, Alexander Howse

Parallel time integration of partial differential equations (PDEs) has become an increasingly important topic during the past several years. Many solution approaches have been developed, particularly for a range of diffusion-dominated problems. An example of one such algorithm is multigrid reduction-in-time (MGRIT). In this talk, I will give an introduction to the MGRIT algorithm and discuss its performance for the advection and heat equations. In particular, I will highlight the poor performance of MGRIT for the advection equation and offer possible strategies for improving the method.

Convergent numerical methods for nonlinear porous media equations

Kim Ngan Le (Monash University)

ngan.le@monash.edu

Collaborators: Jerome Droniou

In this talk, we will consider the non-linear porous media equation which is the standard model of fast diffusion when $0 < m1$. The equation takes the form

$\partial_t u - \Delta(|u|^{m-1}u) = g \quad \text{on } (0,T) \times \Omega,$

with Ω being an open bounded domain in R^d, $d = 1, 2, 3$.

These models are relevant in the description of plasma physic , the flow of a gas as well as a comprehensible fluid through porous media. We will propose a convergent gradient scheme for the problem and show that the weak solution exists. Numerical experiments confirm our theoretical results.

Onsager Coefficient for Collective Diffusion in Binary Melts

Elena Levchenko (University of Newcastle)

Elena.Levchenko@newcastle.edu.au

Collaborators: Alexander Evteev

In this contribution, we derive an analytical expression for the Onsager phenomenological coefficient, $\tilde{L}_{cc}$, for mass transport in a binary melt by making use of the Mori-Zwanzig formalism

$$\tilde{L}_{cc} = \frac{m^2 D_1 D_2}{m^2 D_1 D_2 + c_1 c_2 (m_1 D_1 - m_2 D_2)^2} (1 + \frac{W_{12}}{k_{\mathrm{B}} T})(c_2 D_1 + c_1 D_2). \tag{1}$$

The derived expression allows us to suggest a concept of a binary liquid random alloy ($W_{12} = 0$ or more roughly $|W_{12}|/k_{\mathrm{B}}T \ll 1$) for which the Onsager phenomenological coefficient

$$\tilde{L}_{cc}^{(0)} = \frac{m^2 D_1 D_2}{m^2 D_1 D_2 + c_1 c_2 (m_1 D_1 - m_2 D_2)^2} (c_2 D_1 + c_1 D_2) \tag{2}$$

can be expressed only in terms of: (i) the ratio of the self-diffusion coefficients D_1/D_2, (ii) the ratio of the atomic masses m_1/m_2 ($m = c_1 m_1 + c_2 m_2$), and (iii) the alloy composition c_1 (or c_2, $c_1 + c_2 = 1$). Meanwhile, we demonstrate that the term $W_{12}/k_{\mathrm{B}}T$ is related to a collective energy generation-dissipation effect 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 argue that for binary mixing melts exhibiting chemical ordering (such as Ni-Al melts) the Onsager phenomenological coefficient should typically be $\tilde{L}_{cc} < \tilde{L}_{cc}^{(0)}$ ($W_{12} < 0$), while for binary melts where precursors of liquidliquid demixing are important (such as Cu-Ag melts) the Onsager phenomenological coefficient should be $\tilde{L}_{cc} > \tilde{L}_{cc}^{(0)}$ ($W_{12} > 0$). Furthermore, we show that in thermal equilibrium the Onsager phenomenological coefficient should be within the range $0 \leq \tilde{L}_{cc} \leq 2\tilde{L}_{cc}^{(0)}$, which is constrained by the energy of thermal fluctuations (thermal energy, $k_{\mathrm{B}}T$).

Finally, we employ these theoretical findings for interpretation of recent experimental studies and our molecular dynamics simulations of diffusion kinetics in binary Ni-Al and Cu-Ag melts.

Acknowledgements

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Maximum-norm a posteriori error bounds for parabolic problems

Torsten Linß (Fern Universität in Hagen, Germany)

`torsten.linss@fernuni-hagen.de`

For classical and singularly perturbed parabolic equations, we present maximum norm a posteriori error estimates that, in the singulaly perturbed regime, hold uniformly in the small perturbation parameter. The parabolic equations are discretised in time using the backward Euler method, the Crank-Nicolson method and the discontinuous Galerkin dG(r) method. Both semidiscrete (no spatial discretation) and fully discrete cases will be considered. The analysis invokes elliptic reconsturcions and elliptic a posteriori error estimates. Joint work with Natalia Kopteva (University of Limerick, Ireland).

Comparison of Precipitation and Temperature Trends between Coastal and Inland New South Wales

Shev MacNamara (University of Technology Sydney)

shev.macnamara@uts.edu.au

Collaborators: Joshua Hartigan, Lance M. Leslie

Motivated by the Millennium Drought, the recent water crises in California and Cape Town, and the current drought over much of southern and eastern Australia, this detailed statistical study compares trends in annual wet season precipitation and temperature between a coastal site (Newcastle) and an inland site (Scone). These locations were chosen because the current Australian drought is more pronounced inland than along the coast. In addition to precipitation trends, changes in monthly mean maximum and minimum temperatures are also investigated, as a combination of increasing temperatures and decreasing precipitation places more strain on water resources. Time series of precipitation, monthly mean maximum temperature and monthly mean minimum temperature are grouped into 20-year blocks and bootstrapped to apply permutation tests which compare the 20-year blocks against each other. Precipitation for Scone has dropped significantly over the past 40-years (p-value = 0.07) while Newcastle has had little to no change (p-value = 0.8). Mean maximum temperatures for both sites show a significant increase over the past 40-years (p-values of 0.0008 and 0.058 for Newcastle and Scone, respectively). A similar increase in mean minimum temperature occurred in Newcastle (p-value = 0.015), while Scone showed little change (p-value = 0.79). Wavelet analysis of the Newcastle and Scone time series reveal similar power spectra for precipitation and mean maximum temperature. However, mean minimum temperature power spectra are very different. Newcastle has a statistically significant signal in the 2-7 year period which typically indicates an El-Nino Southern Oscillation (ENSO) climate driver for all three time series, whereas the Scone power spectra has no indication of a definitive driver for mean minimum temperature.

Numerical Solutions to the Nonlinear Electron Diffusion Equation in Dye-Sensitized Solar Cells

Benjamin Maldon*** (University of Newcastle)

benjamin.maldon@uon.edu.au

Dye-Sensitized Solar Cells (DSSCs) have consistently presented a novel solution to the renewable energy problem. Spearheaded by O'Regan and Grätzel's 1991 paper, DSSCs currently see significant academic attention with regards to the choice of semiconductor, the photoactive dye and the electrolyte couple. In spite of this, the area receives comparably less research from a mathematical standpoint. In this talk, we discuss the origin of the nonlinear electron diffusion model and provide numerical solutions obtained by standard finite difference methods, a Runge-Kutta scheme and a new numerical scheme.

Finite volume schemes for multilayer diffusion

Nathan March* (Queensland University of Technology)

nathan.march@hdr.qut.edu.au

Collaborators: Elliot Carr

Diffusion across multiple layers occurs in many industrial, environmental and biological applications e.g. heat conduction in composite materials and groundwater flow across layered soils. Existing numerical methods for solving such problems consider only a limited number of interface conditions and do not carry out stability or convergence analysis. To address these deficiencies, in this talk I present a new finite volume scheme and demonstrate stability and convergence for each of the three classical time discretisation methods: forward Euler, backward Euler and Crank- Nicolson. I show that, consistent with the single-layer problem, the forward Euler scheme is conditionally stable while both the backward Euler and Crank-Nicolson schemes are unconditionally stable. The key contribution of the work is the presentation of a set of sufficient stability conditions for the forward Euler scheme. Here, to ensure stability it is not sufficient that the time step τ satisfies the classical constraint of $\tau \leq h_i^2/(2D_i)$ in each layer (where D_i is the diffusivity and h_i is the grid spacing in the ith layer) as more restrictive conditions can arise due to the interface conditions. The talk concludes with some numerical examples that demonstrate application of the new finite volume method and confirm the theoretical analysis.

Three ways to compute multiport inertance

Geordie McBain (Modelling & Simulation, Memjet North Ryde Pty Ltd)

gmcbain@memjet.com

Collaborators: S. G. Mallinson, B. R. Brown and Tom Gustafsson

When an incompressible fluid is subjected to an impulsive pressure at its boundary, it instantaneously acquires a velocity field which is the gradient of a potential. For a vessel pressurized at an inlet and vented at an outlet, the ratio of the pressure impulse applied to the volumetric flow-rate induced is called the inertance. For a vessel with n ¿ 1 ports, the response is described by an n by n reciprocal-inertance matrix which converts the vector of n port pressures to the corresponding vector of n flow-rates into the ports. The phenomenon of inertance can be derived asymptotically from the short-time solutions of the Navier–Stokes equations and is useful for characterizing transient step-responses in industrial microhydraulic networks.

As an impulsively generated flow has a potential, it is computed by solving a mixed boundary value problem for the Laplace equation. This is conveniently discretized by the Galerkin finite element method. Computing the complete reciprocal-inertance matrix involves as many boundary value problems as there are ports, or rather one less since the conservation of volume implies that the columns of the matrix sum to zero or equivalently one of the ports may be taken as the datum for pressure. The variational boundary value problems have a common bilinear form on the left-hand side but different linear forms on the right, so after discretization can be solved as a single linear system with multiple right-hand side vectors.

The ij-th reciprocal inertance coefficient is defined as the net jump in volumetric flow-rate into the i-th port when the j-th port is given a unit pressure impulse while the others are left at zero pressure. The definition leads to the first way to compute the coefficients: as the surface integral over the port of the normal component of the gradient of the potential. A consideration of the conversion of work into kinetic energy reveals a second formula, involving volume integrals of the scalar products of the fundamental velocity fields. Finally, reinspection of the formula for kinetic energy in the discretized system shows that the corresponding discrete quadratic form has the same matrix as used in the solution for the potentials and that the reciprocal-inertance matrix can be computed by a single evaluation of the quadratic form with the multicolumn potential vector solutions. In the standard Galerkin finite element method with low-order elements convenient for automatically meshing complicated industrial geometries the second and especially third methods are shown to be both simpler to implement and much more accurate and robust with respect to the discretization of the geometry.

Finite volume method for the Geodetic boundary value problem

Matej Medla (Faculty of Civil Engineering STU in Bratislava)

medla@math.sk

Collaborators: Karol Mikula, Robert Cunderlik, Marek Macak

The Earth's gravity field modelling is usually formulated in terms of the geodetic boundary value problems. From the mathematical point of view, it is an exterior oblique derivative BVP for the Laplace equation. We present a numerical solution to this problem on and above the local Earth's topography using the finite volume method (FVM). The Laplace equation is discretized using FVM on non-uniform grids and the oblique derivative boundary condition is treated as a stationary advection equation using an upwind-based FVM. The solution of this system gives the disturbing potential in the whole computational domain including the Earth's surface. Numerical experiments aim to show properties and demonstrate efficiency of the developed FVM approach.

Multi-fidelity sparse girds for uncertainty quantification

Fanzi Meng* (The Australian National University)

u5616659@uds.anu.edu.au

Collaborators: Stephen Roberts

In this work, we look for a surrogate method to provide an approximation of the output of an input-output relationships using as few model evaluations as possible. Simulations are often aimed at exploring the complex relationships between input and output variables, however, when models of real-world systems are complex and the need for multiple realizations, as in uncertainty quantification or optimization, simulations run may be computationally expensive. We aim to make an accurate and efficient surrogate approximation to reduce the cost of the simulation model. A multifidelity approach combine results from accurate and expensive high-fidelity simulations with inexpensive but less accurate low-fidelity simulations in order to achieve accuracy at a reasonable cost. Multi-fidelity methods have been developed on multifidelity Monte Carlo, multifidelity Kriging and multifidelity sparse grids to accelerate the estimation of outputs of high-fidelity models. Our multifidelity approach provides a framework to sample the input parameter space on a sparse grid, and then combine sparse grid interpolation as our surrogate. A multifidelity sparse grid surrogate model is constructed for the Hokkaido-Nansei-Oki tsunami. We demonstrate the experimental results in Okushiri wave flume, which reproduce the maximum value of the time-dependent average tsunami height on top of the Monai zone in Okushiri Island in 1993. We illustrate our approach using a number of uncertain input parameters to quantify the uncertainty in the output of tsunami wave shape and report the achieved savings. Our results consists of both theoretical and numerical parts. In the theoretical part, we discuss the error analysis of convergence on arbitrary dimensions. The numerical results show that for a given accuracy error method can improve efficiency by an order of magnitude.

The forced vibration of a floating elastic plate

Mike Meylan (University of Newcastle)

mike.meylan@newcastle.edu.au

The floating elastic plate is a canonical problem in hydroleasticity which can model a range of application from sea ice to floating airports. I will present a solution to thetime-dependent vibration of a floating elastic plate subject to a transient force. The solution is found in the frequency domain by the eigenfunction matching method. It is shown that the eigenfunction matching in two and three dimensions is almost identical when this symmetry is exploited, and the ease of implementation of this method is demonstrated. The time domain solution is calculated for the case of a Gaussian forcing applied at various points on the plate. The subsequent motion of the plate and its decay due to wave radiation is shown.

Three dimensional free-surface flow over arbitrary bottom topography

Tim Moroney (QUT)

t.moroney@qut.edu.au

Collaborators: Nicholas R. Buttle, Ravindra Pethiyagoda, Scott W. McCue

We consider steady nonlinear free surface flow past an arbitrary bottom topography in three dimensions, concentrating on the shape of the wave pattern that forms on the surface of the fluid. Assuming ideal fluid flow, the problem is formulated using a boundary integral method and discretised to produce a nonlinear system of algebraic equations. The Jacobian of this system is dense due to integrals being evaluated over the entire free surface. To overcome the computational di?culty and large memory requirements, a Jacobian-free Newton Krylov (JFNK) method is utilised. Using a block-banded approximation of the Jacobian from the linearised system as a preconditioner for the JFNK scheme, we find significant reductions in computational time and memory required for generating numerical solutions. These improvements also allow for a larger number of mesh points over the free surface and the bottom topography. We present a range of numerical solutions for both subcritical and supercritical regimes, and for a variety of bottom configurations. We discuss nonlinear features of the wave patterns as well as their relationship to ship wakes.

Use of block Arnoldi method for the efficient numerical solution of nonlinear eigenvalue problems

Hideaki Nagasaka* (Keio University, Japan)

123581321abc@keio.jp

Collaborators: Takashi Nodera

In this talk, we consider approximate solution of nonlinear eigenvalue problem $M(\lambda)x = 0$, where $M(\lambda)$ is a large parameter-dependent matrix and higher-order terms of its Taylor expansion. An operator is used for changing a nonlinear eigenvalue problem to a linear eigenvalue problem. This operator is applied to Arnoldi based scheme. The representation of the operator is the type of block companion matrix. An infinite Arnoldi method, which is advanced version of the Arnoldi method, is usually used to solve the problem. In this method, solutions are reciprocal eigenvalues. We recognize the need for the fast and reliable scheme for solving such systems, inspired by practical as well as cost effective reasons. The main object of this talk is to present a block infinite Arnoldi method with implicit restarting for such problems. Block infinite Arnoldi method is similar to block Arnoldi method, but its procedure to compute eigenvalues is quite different. In order to achieve a satisfactory convergence behavior, Arnoldi method should usually be combined with appropriate restarting strategy. Indeed, when solving the problem with restart, required eigenvalues and eigenvectors are kept while non-required eigenvalues and eigenvectors are removed. Therefore, a size of Hessenberg matrix and eigenvectors are decreased. For this reason, it is observed that this cost-effective with respect to computation time related with orthogonalization as well as required storage resources. Finally, numerical experiments show the efficiency and properties of proposed method.

The Effects of Model Climate Bias on ENSO Variability and Ensemble Prediction

Stacey Osbrough * (CSIRO/Monash University)

stacey.osbrough@csiro.au

Collaborators: Jorgen S. Frederiksen and Carsten S. Frederiksen

New methods are presented for determining the role of coupled ocean-atmosphere model climate bias on the strength and variability of the El Nino – Southern Oscillation (ENSO) and on the seasonal ensemble prediction of El Nino and La Nina events. An intermediate complexity model with a global atmosphere coupled to a Pacific basin ocean is executed in parallel to produce computationally efficient year-long forecasts of large ensembles of coupled flow fields, beginning every month between 1980 and 1999. Firstly, we provide the model with forcing functions that reproduce the average observed annual cycle of climatology of the atmosphere and ocean. We then configure the model to generate realistic ENSO fluctuations. Next, an ensemble prediction scheme is employed which produces perturbations that amplify rapidly over a month. These perturbations are added to the analyses and give the initial conditions for the forecasts. The skill of the forecasts is presented and the dependency on the annual and ENSO cycles determined. Secondly, we replace the forcing functions in our model by the averaged annual cycles of climatology of two state of the art, comprehensive Global Climate Models. The changes in skill of subsequent ensemble forecasts elucidate the roles of model bias in error growth.

A spectral method for the stochastic Stokes equations on the sphere

Joe Peach * (UNSW)

joepeach93@gmail.com

Collaborators: T. Le Gia

We construct numerical solutions to a stochastic Stokes equations on the unit sphere with additive noise. Under certain assumptions, error estimates of the random solution is given. Numerical experiments are carried out to illustrate the theory.

A Finite Element-Volume Method for the Serre Equations

Jordan Pitt * (Australian National University)

jordan.pitt@anu.edu.au

Collaborators: Chris Zoppou, Stephen Roberts

Inundation from water wave hazards such as tsunamis and storm surges poses significant risks to many of our coastal communities. The most efficient method for modelling these hazards and therefore their associated risk is through numerical simulation. Most large scale simulations of tsunamis and storm surges; such as the collaborative effort ANUGA, rely on the Shallow Water Wave equations where wave behavior is primarily determined by nonlinear effects. Recent research has demonstrated that dispersion is also important for the evolution of tsunamis. Therefore, there is a need to develop numerical methods for dispersive equations, such as the Serre equations. Building upon the previous work at the ANU, which developed a hybrid finite volume and finite difference method to solve the Serre equations I have developed an alternative numerical method that combines a finite element and a finite volume method to solve the Serre equations. The developed method has a number of desirable properties; it conserves all the conserved quantities associated with the Serre equations and it is robust. Linear analysis demonstrated that this method was convergent and possessed good dispersion properties. Finally the method was validated against analytic solutions, forced solutions and experimental results.

Generalised smoothing splines in a stochastic setting

Tania Prvan (Macquarie University)

tania.prvan@mq.edu.au

I will introduce generalised smoothing splines in a stochastic setting. I will then look at the special case of fitting exponentials.

A novel shape optimization formulation of the exterior Bernoulli free boundary problem

Julius F. Rabago * (Nagoya University)

jfrabago@gmail.com

Collaborators: Hideyuki Azegami

The exterior Bernoulli problem is rephrased into a shape optimization problem using a new type of objective function called the Dirichlet-data-gap cost function. The first-order shape derivative of the cost function is explicitly determined via the chain rule approach. Then, using the gradient information we formulate an iterative scheme to numerically solve the minimization problem. The feasibility of the proposed method is illustrated through numerical examples.

Non-convex feasibility, Douglas–Rachford, and Lyapunov functions

Björn Rüffer (The University of Newcastle)

bjorn.ruffer@newcastle.edu.au

Feasibility problems are about finding points that are simultaneously in several constraint sets. Such problems are well understood in the case when the constraint sets are all convex, however, many interesting problems are not convex. Still, the Douglas–Rachford algorithm is often observed in practice to find feasible solutions despite the lack of convexity, while it is only proven to do so in the convex case, locally, as well as a small number of non-convex special cases. This talk will demonstrate some recent progress towards global convergence proofs for non-convex problems using Lyapunov functions, which are a tool commonly used in the mathematical systems and control theory community. Lyapunov functions are not only certificates for convergence, they also provide estimates of convergence rates and other stability information. In addition, we will showcase some seemingly simple cases for which still no convergence proofs or Lyapunov functions are known yet.

Multilevel Solvers for The Thin-Plate Spline Saddle Point

Linda Stals (The Australian National University)

linda.stals@anu.edu.au

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. We have discussed various solvers for this saddle point problem over a number of different CTAC conferences. We believe we have now found an efficient robust solver based on a multilevel approach.

Parameter Estimation for Computationally Expensive "Black Box" Models in the Bayesian Framework

Xifu Sun* (The Australian National University)

xifu.sun@anu.edu.au

Expensive "Black Box" models are used in many fields of science, and the idea of reducing cost while keeping the efficiency becomes crucial nowadays. Different Monte Carlo methods are used to achieve such goal as running models on several sample points rather than the whole space; however, Markov Chain Monte Carlo method (MCMC) is an often used yet not most efficient method for inverse problems. Tunable Diode Laser Absorption Spectroscopy (TDLAS) is one of the inverse problems, and our interest is comparing the efficiency of MCMC with Quasi Monte Carlo method (QMC) on TDLAS methods.

Competitive combustion reactions in two dimensions

Simon Watt (UNSW, Canberra)

simon.watt@adfa.edu.au

Collaborators: Simon Watt, Zhejun Huang and Harvinder Sidhu

We consider a system of reaction-diffusion equations describing the combustion dynamics and the reaction is assumed to undergo two competitive reaction, one which is exothermic and the other which is endothermic. The one dimensional model has been shown to exhibit complex behaviour, from propagating combustion waves with a constant speed to period doubling cascades and the possibility of chaotic wave speeds. In this study, we extend the combustion model from one to two dimension by exploring a model with no heat loss in an insulated strip and axially symmetric spread. In particular, we compare and contrast the behaviour of the systems in one and two dimensions. We consider a system of reaction-diffusion equations describing the combustion dynamics and the reaction is assumed to undergo two competitive reaction, one which is exothermic and the other which is endothermic. The one dimensional model has been shown to exhibit complex behaviour, from propagating combustion waves with a constant speed to period doubling cascades and the possibility of chaotic wave speeds. In this study, we extend the combustion model from one to two dimension by exploring a model with no heat loss in an insulated strip and axially symmetric spread. In particular, we compare and contrast the behaviour of the systems in one and two dimensions.

Numerical Investigation and Modelling of the Venous Injection of Sclerosant Foam

Kaichung Wong * (The University of Sydney)

kwon6774@uni.sydney.edu.au

Collaborators: Steven Armfield and Nicholas Williamson

Sclerosant foam, that is a mixture of a surfactant liquid and air, is injected directly into varicose veins as a treatment that causes the vein to collapse. The motivation of this investigation is to develop a model that will allow the medical specialist to visualise how the sclerosant foam will interact with the blood and behave within the vein. The process is simulated using a multiphase computational fluid dynamics model with three approaches; the sclerosant foam considered as a bulk non – Newtonian Power Law viscosity liquid; as a two – phase liquid; and as a two – phase non – Newtonian Power Law viscosity liquid. The last two approaches are also coupled with a Population Balance Model (PBM) to predict the bubble size distribution within the flow field. All cases are based on an Eulerian – Eulerian multiphase model. The best results obtained were with the two phase non – Newtonian Power Law viscosity liquid approach where the computational model demonstrated similar flow characteristics and flow features to an available set of experimental results. The mixing layers between the sclerosant foam and the ambient fluid and the sclerosant liquid and the ambient fluid are correctly predicted in the two – phase non – Newtonian Power Law viscosity liquid model whereas no mixing layers are predicted by the other two approaches. The two-phase non – Newtonian Power Law viscosity approach also predicted the sclerosant liquid coverage on the vein wall and the bubble size distribution within the vein, which is of interest to medical specialists allowing them to assess the treatment feasibility and safety before treating the patients.

The application of sparse grid quadrature in solving stochastic optimization problems

Yuancheng Zhou * (The Australian National University)

yuancheng.zhou@anu.edu.au

Collaborators: Markus Hegland

Stochastic optimization is a useful tool in decision making and has a wide variety of applications. The objective function of a stochastic optimization problem is usually an expectation of some functions of the decisions and the uncertainties. The goal is to optimize this expectation and find the best decisions that will perform well on average. If the number of the uncertainties is large, then the expectation will become a high dimensional integral. We will encounter the curse of dimensionality when we approximate the objective function as a consequence. Thus, how to compute these expectations efficiently is the key to solve complex stochastic optimization models. In this talk, the sparse grid quadrature will be introduced and applied to solve some stochastic optimization models.

Participants

Riya Aggarwal
University of Newcastle
Riya.Aggarwal@uon.edu.au

Mohamed Al-Sultani
Massey University
M.Al-Sultani@massey.ac.nz

Steven Armfield
Sydney University
steven.armfield@sydney.edu.au

David Allingham
University of Newcastle
david.allingham@newcastle.edu.au

Layth Awin
The University of Sydney
lawi8820@uni.sydney.edu.au

Abhishek Bhardwaj
Australian National University
Abhishek.Bhardwaj@anu.edu.au

Elliot Carr
Queensland University of Technology
elliot.carr@qut.edu.au

Vivien Challis
The Unversity of Queensland
vchallis@maths.uq.edu.au

Hanz Martin Cheng
Monash University
hanz.cheng@monash.edu

Gopikrishnan Chirappurathu Remesan
Monash University,
gopikrishnan.chirappurathuremesan@monash.edu

Barry Croke
Australian National University
barry.croke@anu.edu.au

Neil Dizon
The University of Newcastle
neilkristofer.dizon@uon.edu.au

Jerome Droniou
Monash University
jerome.droniou@monash.edu

Robert Eymard
Université Paris-Est Marne-la-Vallée
Robert.Eymard@u-pem.fr

Lishan Fang
Australian National University
Lishan.Fang@anu.edu.au

Fillipe Georgiou
University of Newcastle
fillipe.georgiou@uon.edu.au

Brendan Harding
University of Adelaide
brendan.harding@adelaide.edu.au

Markus Hegland
Australian National University
markus.hegland@anu.edu.au

Feng-Nan Hwang
National Central University, Taiwan
hwangf@math.ncu.edu.tw

David Jenkins
University of Newcastle
david.jenkins@newcastle.edu.au

Zlatko Jovanoski
UNSW Canberra
z.jovanoski@adfa.edu.au

Vesa Kaarnioja
University of New South Wales
v.kaarnioja@unsw.edu.au

Matthias Kabel
Fraunhofer Institute for Industrial Mathematics
matthias.kabel@itwm.fraunhofer.de

Balaje Kalyanaraman
University of Newcastle
Balaje.Kalyanaraman@uon.edu.au

Amandeep Kaur
Indian Institute of Technology Ropar
amandeep.kaur@iitrpr.ac.in

Andreas Kromik
University of Newcastle
Andreas.Kromik@uon.edu.au

Oliver Krzysik
Monash University
oliver.krzysik@monash.edu

Frances Kuo
University of New South Wales
`f.kuo@unsw.edu.au`

Bishnu Lamichhane
University of Newcastle
`blamichha@gmail.com`

Kim Ngan Le
Monash University
`ngan.le@monash.edu`

Quoc Thong Le Gia
University of New South Wales
`qlegia@unsw.edu.au`

Elena Levchenko
University of Newcastle
`Elena.Levcheno@newcastle.edu.au`

Torsten Linß
Fern Universität in Hagen, Germany
`torsten.linss@fernuni-hagen.de`

Shev MacNamara
University of New South Wales
`shev.mac@gmail.com`

Benjamin Maldon
University of Newcastle
`benjamin.maldon@uon.edu.au`

Nathan March
Queensland University of Technology
`nathan.march@hdr.qut.edu.au`

Geordie McBain
Modelling & Simulation, Memjet North Ryde Pty Ltd
`gmcbain@memjet.com`

Matej Medla
Faculty of Civil Engineering STU in Bratislava
`medla@math.sk`

Fanzi Meng
The Australian National University
`u5616659@uds.anu.edu.au`

Mike Meylan
University of Newcastle
`mike.meylan@newcastle.edu.au`

Tim Moroney
QUT
`t.moroney@qut.edu.au`

Mary Myerscough
University of Sydney
mary.myerscough@sydney.edu.au

Hideaki Nagasaka
Keio University, Japan
123581321abc@keio.jp

Stacey Osbrough
CSIRO/Monash University
stacey.osbrough@csiro.au

Joe Peach
UNSW
joepeach93@gmail.com

Jordan Pitt
ANU
jordan.pitt@anu.edu.au

Andreas Prohl
University of Tuebingen, Germany
prohl@na.uni-tuebingen.de

Tania Prvan
Macquarie University
tania.prvan@mq.edu.au

Julius Fergy Rabago
Nagoya University
jfrabago@gmail.com

Björn Rüffer
The University of Newcastle
bjorn.ruffer@newcastle.edu.au

Stephen Roberts
Australian National University
stephen.roberts@anu.edu.au

Vera Roshchina
University of New South Wales
v.roshchina@unsw.edu.au

Ian Sloan
University of New South Wales
i.sloan@unsw.edu.au

Linda Stals
The Australian National University
linda.stals@anu.edu.au

Xifu Sun
The Australian National University
xifu.sun@anu.edu.au

Thanh Tran
University of New South Wales
thanh.tran@unsw.edu.au

Ian Turner
School of Mathematical Sciences, Queensland University of Technology
i.turner@qut.edu.au

Simon Watt
ADFA
simon.watt@adfa.edu.au

Kaichung Wong
The University of Sydney
kwon6774@uni.sydney.edu.au

Yuancheng Zhou
Australian National University
yuancheng.zhou@anu.edu.au

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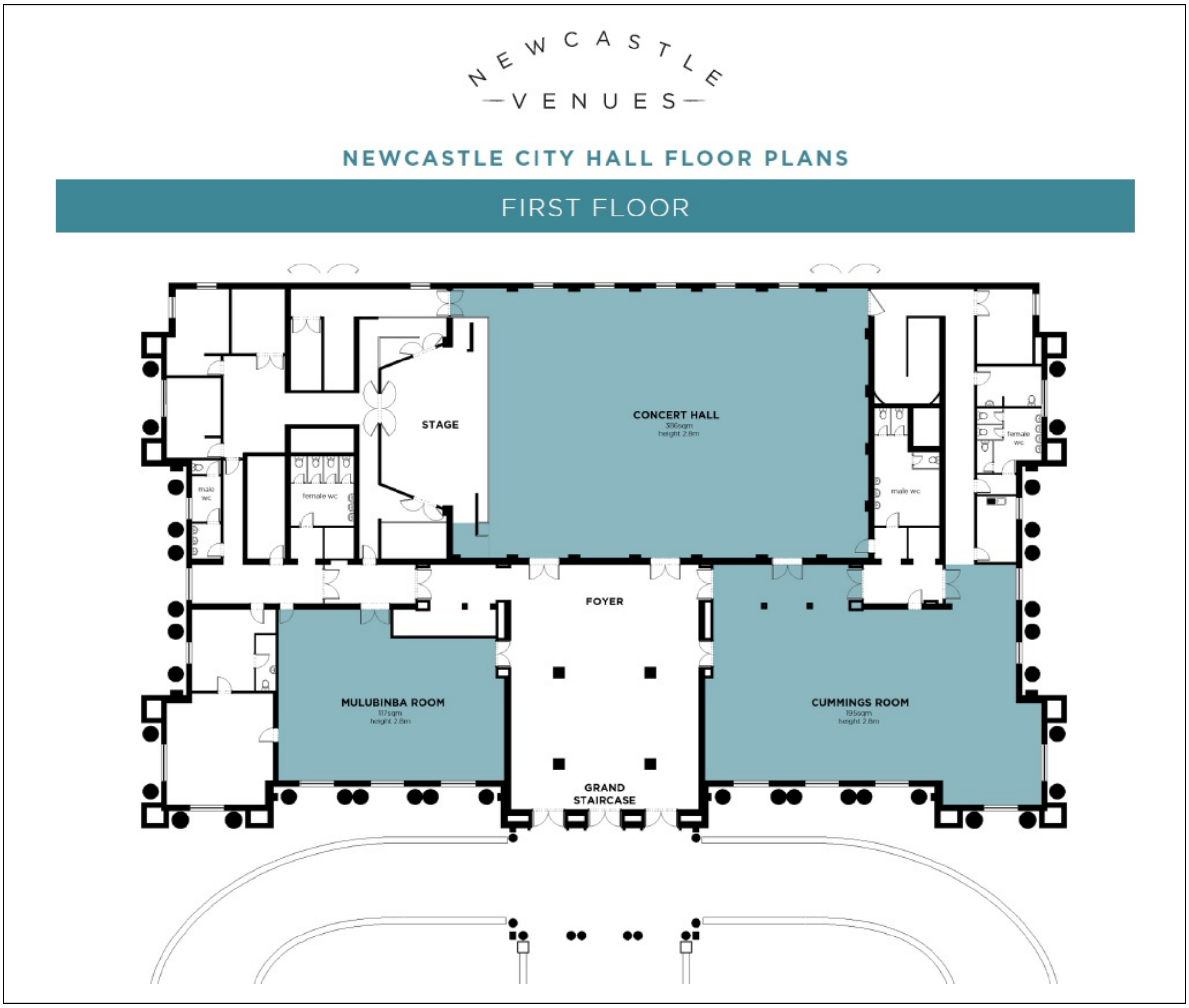
The City of Newcastle

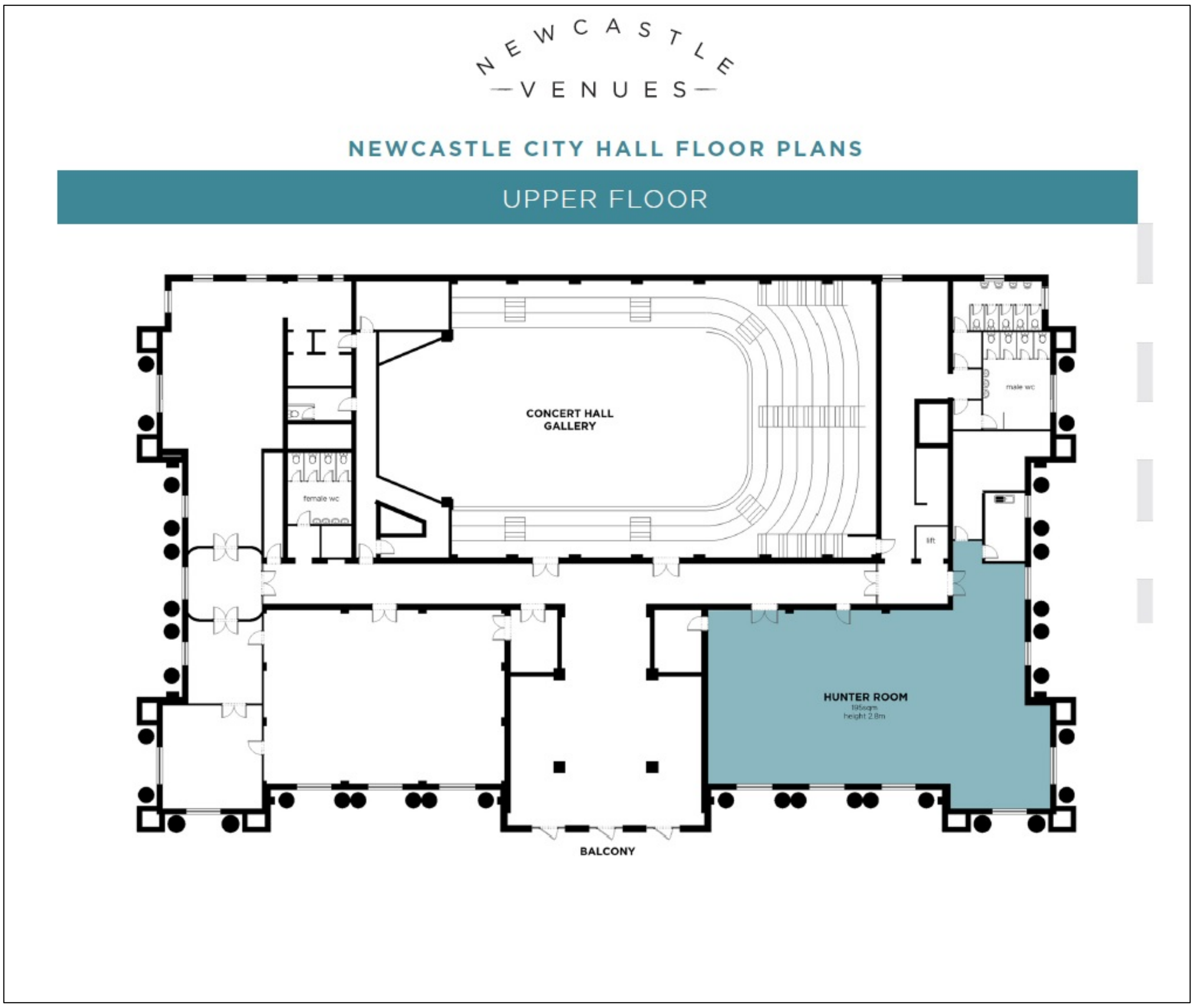
1ST FLOOR

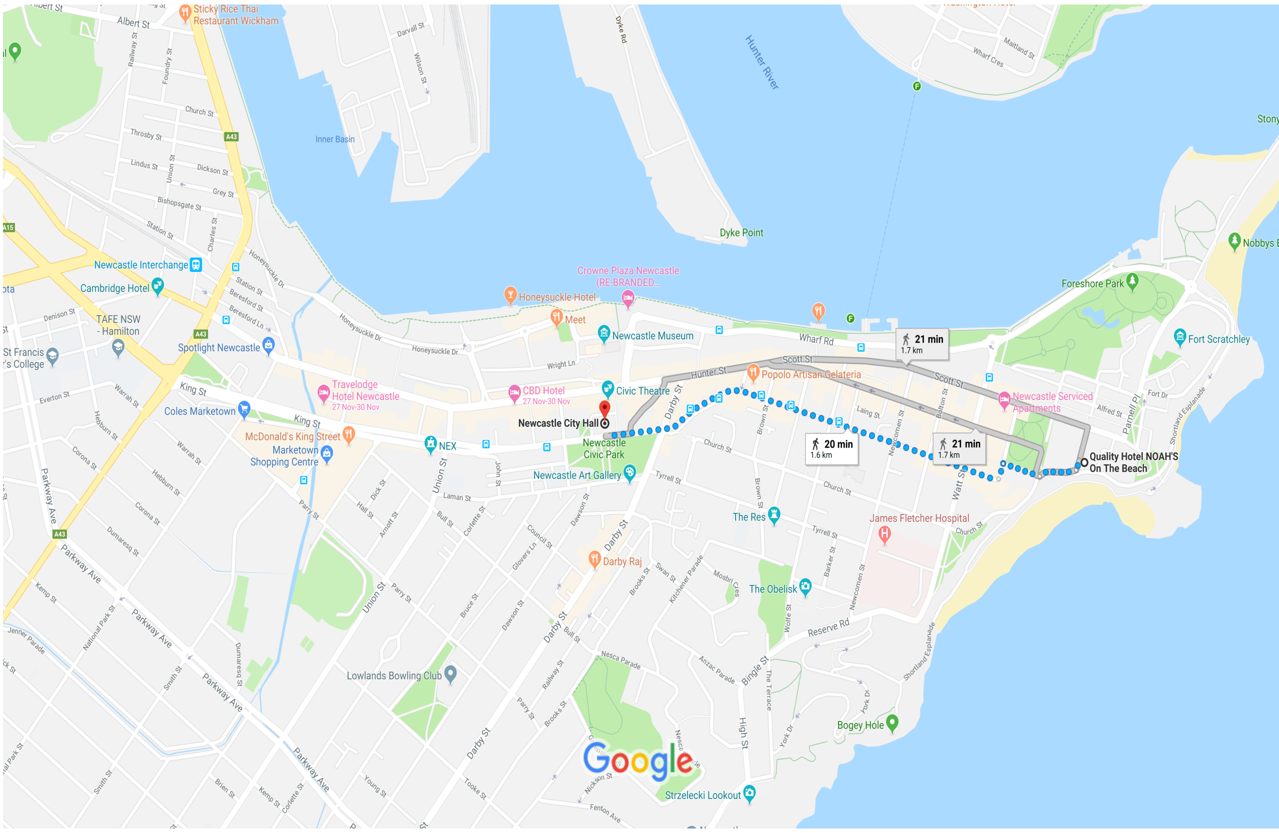
The 1st Floor of Newcastle City Hall is home to the Concert Hall, Cummings Room and Mulunbinba Room.



UPPER FLOOR

The Upper Floor of Newcastle City Hall features the Hunter Room and access to the Concert Hall Gallery.

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Newcastle Art Gallery
NEX
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