CTAC2010
The 15th Biennial Computational Techniques and Applications Conference

28th Nov–1st Dec 2010
University of New South Wales
Sydney, NSW, Australia

CTAC2010 Conference Abstracts
Quoc Thong Le Gia & Thanh Tran (Editors)

Contents

Welcome

We are pleased to host the 15th Biennial Computational Techniques and Applications Conference (CTAC2010) at the School of Mathematics and Statistics of the University of New South Wales, Sydney, Australia.

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 2008 at the Mathematical Sciences Institute, Australian National University.

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 hope you will enjoy the conference and meet many interesting colleagues.

Sponsors

- School of Mathematics and Statistics, University of New South Wales
- Centre of Excellence for Mathematics and Statistics of Complex Systems
- Australian Mathematical Sciences Institute
- Australian and New Zealand Industrial and Applied Mathematics
- CSIRO Mathematical and Information Sciences

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Information

Conference venue

The conference is hosted by the School of Mathematics and Statistics at the University of New South Wales, Kensington campus. There is a map at the back of this booklet which will be used for reference throughout this text. On the map, the School is located at map coordinate H13.

The registration and information desk will be located at the entrance of the Webster B lecture theatre (map coordinate G15, upstairs).

The invited presentations will take place in Webster B lecture theatre. The contributed presentations will take place concurrently in the Webster B, Webster 250, Webster 251 lecture rooms.

The public lecture will take place in Physics Main Theatre, map coordinate K14.

Coffee breaks will be held close to Webster B lecture theatre.

The participants are on their own for lunches. There are plenty of places to eat on campus. On campus map, the coordinates for those restaurants and cafeteria are E6, G6, F12, F15, K17, D20.

Presentations

Each lecture theatre is equipped with a desktop computer running Windows, with mouse, keyboard, USB ports, and Internet connection. There is also a fixed data projector (connected to the desktop) and a projection screen. There are also blackboards.

All talks are 15 minutes long, plus 5 minutes for questions and discussion. The session chair will give you a signal when you have 5 minutes remaining. Please do not exceed your time.

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 desktop computer before your talk.

The desktop in the lecture theatre can display Powerpoints documents but we cannot guarantee that all fonts are available. Note that postscript files cannot be displayed.

If you require access to other software packages or other audio-visual equipments please talk to the organizers 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 organizers to test the connection well before your presentation.

Internet access

Wireless Internet access is available for all participants through the UNIWIDE network. Upon registration you will receive a personal login and password with which you can connect to UNIWIDE.

Those who do not have laptop available (or do not want to use it) can also get internet access in the student PC laboratory M020 at the Mezzanine level (which is the ground level) of the Red Centre. The lab is open from 8am until 9pm. A login and password will be provided at the registration desk.

Social events

On Sunday evening we have a welcome reception at 6:00pm. It will be held at Roundhouse, Courtyard Bar. The map coordinate of Roundhouse is E6.

The conference dinner will be held on Tuesday evening at 6:30pm, at Giovanna Italian Restaurant, 285 Anzac Parade, Kingsford (outside campus).

Travel to and from the airport

- *Taxi:* The journey from the University of New South Wales (UNSW) to the airport takes 15 to 20 minutes and costs around AUD $35.
- *Bus:* The route 400 bus will take you from UNSW to the airport. The trip takes about 40 minutes and costs about AUD $4.20. There are 2 bus stations which you can take bus 400: one is on ANZAC parade, opposite the main gate of UNSW and the other is on High St., opposite Lowy Cancer Research Center. Please make sure to ask the bus driver that the bus is going to the airport.
- *Train:* If you are staying in the City near Central Station or one of the City Circle stations, the Airport Link train runs regularly and takes about 15 minutes to reach the airport from Central Station. The fare is approximately AUD $15.

Travel around Sydney

Sydney has an extensive public transport network involving trains, buses and ferries. There is a lot of information on the Transport Infoline webpage `http://www.131500.info/` or `http://www.sydneybuses.info/`

Note that you have to purchase a prepaid ticket (from any newsagents or any shop displaying the purple PREPAID symbol) before boarding any express or limited stop bus service (e.g. bus route 891 and metrobus 10) and bus in the City (e.g. Eddy Ave, George St., etc) between 7am and 7pm on weekdays.

UNSW is situated on several bus routes. From Central Station catch the 891 Express bus or routes 391, 393, 395. The journey takes around 15 minutes on the express bus and around 25 minutes on other routes. The route 10 metrobus is a limited stop service that passes the University of New South Wales. You can catch it from Railway Square, and a number of stops of George St., Park St. or Elizabeth St. From Circular Quay you can catch the 392, 394, 396, X94, L94 towards UNSW.

Dining

There are many restaurants near UNSW.

- ANZAC Parade: Walk South along ANZAC parade from UNSW to find a number of inexpensive Asian, Italian restaurants.
- Randwick: Walk East up High Street pass the Prince of Wales Hospital and turn left into Belmore Rd. There are a number of Asian, Mexican, Italian restaurants along Belmore and Alison Rd.
- The Spot: Walk East up High Street pass the Prince of Wales Hospital and turn right into Belmore Rd then Perouse Rd. There are many cafeterias, bars, restaurants and a cinema.

Program

Sunday Nov 28th, 2010

6:00–8:00 pm	Opening registration/Welcome reception (Round House, Courtyard Bar).

Monday Nov 29th, 2010

8:00–8:45	Registration		
8:45–9:00	Opening		
9:00–10:00	Engquist (p. 12) - invited lecture (Webster B)		
	CFD (Webster B)	Industrial Appl (Webster 250)	Data Analysis (Webster 251)
10:00–10:20	Li (p. 42)	Luangwilai (p. 44)	Pardy (p. 52)
10:20–10:40	Smith (p. 58 bottom)	Mat Isa (p. 46)	Grainger (p. 31)
10:40–11:00	J. Frederiksen (p. 30)	Anderssen (p. 18)	C. Frederiksen (p. 29)
11:00–11:20	Morning tea		
	CFD (Webster B)	Computational Math (Webster 250)	Biomathematics (Webster 251)
11:20–11:40	S. Roberts (p. 54)	Shepherd (p. 56)	Motyer (p. 48)
11:40–12:00	Djanali (p. 26)	Hawkins (p. 33)	J. Song (p. 59)
12:00–12:20	Mungkasi(p. 48)	Le Gia (p. 40 bottom)	Jing (p. 36)
12:20–12:40	Harvie (p. 31)	Brown (p. 22)	Belward (p. 20)
12:40–1:40	Lunch		
1:40–2:40	Knackstedt (p. 12) - invited lecture (Webster B)		
	CFD (Webster B)	Computational Math (Webster 250)	Optimisation (Webster 251)
2:40–3:00	Zidikheri (p. 67)	Stals (p. 60)	Smith (p. 58 top)
3:00–3:20	Kitsios (p. 38)	L. Song (p. 59)	Mawengkang (p. 46)
3:20–3:40	O'Kane (p. 51)	Carr (p. 23)	Tarnopolskaya (p. 62)
3:40–4:00	Afternoon tea		
	CFD (Webster B)	Computational Math (Webster 250)	HPC (Webster 251)
4:00–4:20	Biscombe (p. 21)	Nichols (p. 50)	Moroney (p. 47)
4:20–4:40	Khanal (p. 37)	Enting (p. 28)	Engwirda (p. 27)
4:40–5:00	Berry (p. 21)	Taheri (p. 57)	Fang (p. 28)
5:00–5:20		Kosowski (p. 39)	Thanigaivelan (p. 63)
6:00–8:00	Jamie Sethian (p. 14) - Public lecture (Physics Main Theatre - map ref. K14)		

Tuesday Nov 30th, 2010

9:00–10:00	Cornwell (p. 11) - invited lecture (Webster B)		
	CFD (Webster B)	Optimisation (Webster 250)	Biomathematics (Webster 251)
10:00–10:20	Hattori (p. 32)	Prvan (p. 53)	Nasution (p. 49)
10:20–10:40	Zecevic (p. 67)	Tappenden (p. 61)	Hegland (p. 34)
10:40–11:00	Wiryanto (p. 64)		Sunkara (p. 60)
11:00–11:20	Morning tea		
	CFD (Webster B)	Computational Math (Webster 250)	Biomathematics (Webster 251)
11:20–11:40	Dittko (p. 25)	Pham (p. 53)	Mallet (p. 45)
11:40–12:00	Williamson (p. 64)	Le Gia (p. 41)	Bagher Oskouei (p. 19)
12:00–12:20	Armfield (p. 17)	Shiroishi (p. 56)	Samsuzzoha (p. 55)
12:20–12:40	Xu (p. 65)	Kuroiwa (p. 39)	Delia Nova (p. 24)
12:40–1:40	Lunch		
1:40–2:40	Kuo (p. 13) - invited lecture (Webster B)		
	Industrial Appl (Webster B)	Computational Math (Webster 250)	Engineering Computations (Webster 251)
2:40–3:00	Alam (p. 16)	Andrew (p. 18)	Sharples (p. 55)
3:00–3:20	Huda (p. 35)	Chen (p. 23)	Madadi (p. 45)
3:20–3:40	Dogan (p. 27)	Tarnopolskaya (p. 61)	Kha (p. 37)
3:40–4:00	Afternoon tea		
	High Dimensional Probs (Webster B)	Computational Math (Webster 250)	Data Analysis (Webster 251)
4:00–4:20	Newsam (p. 50)	Yang (p. 65)	Yu (p. 66)
4:20–4:40	Brauchart (p. 22)	Farmer (p. 29)	Ong (p. 51)
4:40–5:00	Baldeaux (p. 20)	Le Gia (p. 40 top)	Sidhu (p. 57)
5:00–5:20	Leopardi (p. 41)	Al-Lawatia (p. 16)	Hay (p. 33)
6:30–8:30	Conference dinner Giovanna Italian Restaurant, 285 Anzac Parade, Kingsford		

Wednesday Dec 1st, 2010

9:00–10:00	Scheichl (p. 13) - invited lecture (Webster B)		
	CFD (Webster B)	Computational Math (Webster 250)	Biomathematics (Webster 251)
10:00–10:20	Mungkasi (p. 49)	D. Roberts (p. 54)	Watanabe (p. 63)
10:20–10:40	Back (p. 19)	Otani (p. 52)	Liu (p. 43)
10:40–11:00	Dallaston (p. 24)	Hashentuya (p. 32)	Hsieh (p. 34)
11:00–11:20	Morning tea		
11:20–12:20	Durbin (p. 11) - invited lecture (Webster B)		
12:20–12:35	Discussion about CTAC proceedings		
12:35–12:40	Conference close		

Abstracts of invited presentations

Large Computational and Algorithmic Challenges of the Square Kilometre Array

Tim Cornwell
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Over much of its 80 year history, radio astronomy has been enabled by and dependent on three technologies: digital signal processing, computing, and networking technologies. By the end of this decade, radio astronomers working in an international consortium will have built the world's largest, most sensitive, fastest radio telescope, the Square Kilometre Array. The SKA will be one of the foremost scientific instruments in the world, addressing some of the most important questions in astrophysics and cosmology. The SKA will naturally stress and stretch the state of the art in the three technology areas mentioned above. One of the most notable technical aspects of the SKA is the very large data rate - exceeding 10 Pbit/s over long-distance networks into the digital signal processing chain, requiring about 1 Exaflop/s for processing into images, and producing 1 Exabyte of science data per week. The data rate raises many issues throughout the entire system design. I will concentrate on the interaction between the computing architecture and the physics and algorithmics of the measurement process.

Tuesday 9:00–10:00 Webster B

Turbulent Flow Through a Serpentine Channel

Paul Durbin
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The serpentine geometry is meant to isolate the influence of curvature on turbulence. Periodicity is imposed between inlet and exit and a fully developed flow field develops in our direct numerical simulation. The duct is rotated to examine the combined effects of curvature and rotation. The theoretical framework will be sketched. Stabilizing and destabilizing influences of curvature and rotation are seen in the DNS data. Large, but quite weak, streamwise vortices form due to convex curvature; but they break up under rotation, possibly because rotation destroys the symmetry between the two bends of the serpentine. Within the bends turbulent intensities are enhanced or suppressed roughly in accord to theory. Particles are tracked in the flow and some rather interesting distributions of particle accumulation are seen. Light particles acculumlate somewhat along the walls. It is unclear whether turbophoresis plays a role, or whether this is a balance of centrifugal acceleration and turbulent dispersion. Heavy particles form into jets, leaving the inner wall, and bands of concentration are caused by multiple reflections from the outer wall. The concentration bands spread by turbulent mixing. Standard drag formulas for one-way coupling are used for the particle trajectories. The domain is partitioned geometrically, so the high concentrations cause the particle tracking to be poorly load balanced.

Wednesday 11:20–12:20 Webster B

Multiscale Methods for Wave Propagation

Bjorn Engquist
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We will give a brief overview of multiscale modeling for wave equation problems and then focus on two techniques. One is the heterogeneous multiscale method applied to problems with oscillatory velocity fields. In this technique calculations in time domain on a refined grid is performed on small subsets of the computational domain to achieve efficiency. The other technique is a new class of sweeping preconditioners for frequency domain simulation with variable coefficients resulting in computational procedures that essentially scale linearly even in the high frequency regime.

Monday 9:00–10:00 Webster B

The Digital Materials Laboratory

Mark Knackstedt
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One of the main obstacles to real progress in the science of complex real world materials has been the need to accurately characterise material structure and thereby to predict properties of materials in three dimensions. We describe the development of a new quantitative numerical laboratory approach to the study of complex real world materials in 3D. A first part incorporates the development and integration of experimental 3D imaging facilities for characterizing materials at multiple scales. A second part is the development of computational infrastructure for image reconstruction, phase identification, multiscale mapping, 3D visualisation, structural characterisation and prediction of physical properties of material properties from digitised 3D images. We describe examples where the ability to quantitatively measure and characterize the structure and properties of complex materials in 3D has impacted on applied sciences including materials design and bone health diagnosis. We also describe proven commercial applications of the technology in the resources sector.

Monday 1:40–2:40 Webster B

Lifting the Curse of Dimensionality - Quasi Monte Carlo Methods for High Dimensional Integration

Frances Kuo
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High dimensional problems, that is, problems with a very large number of variables, are coming to play an ever more important role in applications. These include, for example, option pricing problems in mathematical finance, maximum likelihood problems in statistics, and porous flow problems in computational physics. High dimensional problems pose immense challenges for practical computation, because of a nearly inevitable tendency for the costs of computation to increase exponentially with dimension: this is the celebrated "curse of dimensionality". In this talk I will give an introduction to "quasi-Monte Carlo methods" for tackling high dimensional integrals, with a focus on "lattice rules", and discuss the challenges that we face while attempting to lift the curse of dimensionality.

Tuesday 1:40–2:40 Webster B

Multilevel Simulation under Uncertainty

Robert Scheichl
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The quantification of uncertainty in groundwater flow plays a central role in the safety assessment of radioactive waste disposal and of CO2 capture and storage underground. Stochastic modelling of data uncertainties in the rock permeabilities lead to elliptic PDEs with random coefficients. A typical computational goal is the estimation of the expected value or higher order moments of some relevant quantities of interest, such as the effective permeability or the breakthrough time of a plume of radionuclides. Because of the typically large variances and short correlation lengths in groundwater flow applications, methods based on truncated Karhunen-Loeve expansions are only of limited use and Monte Carlo type methods are still most commonly used in practice. To overcome the notoriously slow convergence of conventional Monte Carlo, we formulate and implement novel methods based on (i) deterministic rules to cover probability space (Quasi-Monte Carlo) and (ii) hierarchies of spatial grids (multilevel Monte Carlo). It has been proven theoretically for certain classes of problems that both of these approaches have the potential to significantly outperform conventional Monte Carlo. A full theoretical justification that the groundwater flow applications discussed here belong to those problem classes are under current investigation. However, experimentally our numerical results show that both methods do indeed always clearly outperform conventional Monte Carlo even within this more complicated setting, to the extent that asymptotically the computational cost is proportional to the cost of solving one deterministic PDE to the same accuracy.

Wednesday 9:00–10:00 Webster B

In Pursuit of Interfaces - Inkjet Plotters, Coating Rollers, Semiconductors, Retinopathy, and Chemical Pathways

Jamie Sethian
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Propagating interfaces occur in a wide variety of settings, and include ocean waves, burning flames, and material boundaries. Less obvious boundaries are equally important, and include iso-intensity contours in images, handwritten characters, and shapes against boundaries. In addition, some static problems can be recast as advancing fronts, including robotic navigation and finding shortest paths on contorted surfaces. One way to frame moving interfaces is to recast them as solutions to fixed domain Eulerian partial differential equations, and this has led to a collection of PDE-based techniques, including level set methods, fast marching methods, and ordered upwind methods. These techniques easily accommodate mergingboundaries and the delicate 3D physics of interface motion. In many settings, they been proven valuable. In this talk, we will focus on scientific and engineering applications of these techniques. This will include "How do home inkjet plotters work?". "What happens when my faucet drips?" "How can we guide chemical probes through complex materials?". "How are semiconductors built?". And, "How can we automate the early detection of eye disease?".

Monday 6:00–8:00 Physics Main Theatre

Abstracts of contributed presentations

CFD Modeling of Oxygen Injection in EAF Steelmaking

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In Electric Arc Furnace (EAF) steelmaking, scrap metal is melted by using an electric arc and oxy-fuel burner inside the furnace. After melting the molten metal is purified by blowing oxygen supersonically into the molten metal. But this process results in splashing of the liquid melt on the furnace wall which causes wearing of refractories, skulling on the mouth of the vessel and loss of production. In the present study, a computational fluid dynamics (CFD) model of supersonic oxygen injection in EAF steelmaking furnace has been developed in two parts. At first the modelling of supersonic jet characteristics inside the steelmaking furnace has been performed considering only the gas phase. The gas jet is found to decay at slower rate at steelmaking temperature compared with the room temperature. Then the modelling of jet impinging on liquid surface and wall splashing has been carried out. The Eulerian-Eulerian approach was used for simulating the multiphase flow and the volume of fluid (VOF) method was used to calculate the sharp interface between gas and liquid. The CFD results are then validated against the existing experimental data and there is a good agreement between the CFD and experimental results. This model will be helpful in calculating the droplet generation rate at different operating conditions (lance height, flow rate, lance angle) of EAF steelmaking and in choosing the condition to produce less splash.

Tuesday 2:40–3:00 Webster B

A Finite Volume Characteristic Method for Multi-Dimensional Advection Diffusion Equations

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We develop a characteristic method for the solution of the transient advection diffusion equations in multiple space dimensions. This method uses finite volume test functions within the framework of the Eulerian Lagrangian localized adjoint methods (ELLAM). It therefore maintains the advantages of this class of methods which include global mass conservation as well as natural treatment of all types of boundary conditions. However, it differs from previous finite volume methods in that class in the treatment of the mass storage integral at the previous time step. The new treatment is suitable for orthogonal grids and results in a simple algorithm based on backward tracking which retains mass conservation at no additional expenses in terms of accuracy or CPU consumption. Numerical experiments are presented which illustrate the strong potential of the method.

Tuesday 5:00–5:20 Webster 250

Transition to Unsteady Natural Convection Flow of Water in Open Enclosures

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The present study is concerned with unsteady natural convection flow in a two dimensional fully open enclosure for both transient and steady-state ow. The left hand vertical wall of the enclosure is heated and the right hand facing boundary is open, with the top and bottom boundaries insulated. Buoyancy-driven flows of this type, due to heat transfer in open enclosures, occur in many applications; for instance, horizontal transport in water bodies, stratification process in thermosyphon systems, heating and cooling of containers in food industries, crystal growth procedures and in pipes joining reservoirs of fluids with different temperature. In these applications, the buoyancy is unsteady which is of fundamental interest. The numerical solutions will be obtained by solving the Navier-Stokes equations and the temperature transport equation on a non-staggered grid using an unsteady second-order finite-volume scheme with a pressure correction equation used to simultaneously provide an update for the pressure field and enforce the divergence free condition. Results will be presented for Rayleigh numbers in the rang 1 x 105 to 1 x 1010 with Prandtl number 7.0. It will be shown that the ow transits from steady to unsteady, at full development, with increasing Rayleigh number from 1 x 105 to 1 x 1010.

Tuesday 12:00–12:20 Webster B

Information Recovery from Near Infrared Spectra

Bob (Robert) Anderssen
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When the complexity of a situation is such that it is not possible or appropriate to formulate a mathematical model, a popular alternative is calibration-and-prediction (CAP). Indirect measurements (e.g. near-infrared (NIR) spectra) of the phenomenon (e.g. wheat) are recorded for a large number of samples in conjunction with corresponding laboratory measurements of the property of interest (e.g. protein content). This set of dual measurements defines the ”calibration data”. In the calibration step, a (linear) relationship, that defines the property as a function of the indirect measurements, is fitted to the calibration data. This calibration relationship then becomes the ”predictor” for the property for the indirect measurements performed on subsequent samples. The need to perform further laboratory measurements of the property is thereby circumvented. The calibration step is normally performed using a partial least squares, support vector machine or neural network methodology, to generate a predictor of the property using the measured spectra. Independently, because of the high accuracy with which NIR spectra are recovered, using computer controlled instrumentation, it has been established that derivative spectroscopy techniques can be utilised to explore differences in molecular structure of barley mutants. This leads naturally to the idea of performing the calibration step to generate a predictor of the property using fourth derivatives.

Monday 10:40–11:00 Webster 250

Inverse Sturm-Liouville Problems: Some Recent Developments

Alan Andrew
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This paper considers numerical methods for obtaining information on the potentials of Sturm-Liouville operators from spectral data. It describes some recent work of the author and others on methods using an asymptotic correction technique of Paine, De Hoog and Anderssen, and compares these methods with other available methods. Work more recent than the author's paper in Inverse Problems 22 (2006) 2069-2081 is emphasized. Topics covered include a discussion of difficulties arising from the scarcity of accurate data in physical applications, a preview of some work in progress, and some suggestions for future work.

Tuesday 2:40–3:00 Webster 250

Numerical Solution to an Ill-Posed Stefan Problem

Julian Back
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The Stefan problem for freezing a supercooled liquid (or melting a superheated solid) is known to be ill-posed with certain initial conditions leading to finite-time blow-up. We present numerical solutions to this problem, with emphasis on near blow-up behaviour. Further, a problem that involves surface tension is also considered, and the results discussed in the context of melting a very small ice-ball.

Wednesday 10:20–10:40 Webster B

Implementation of a Hybrid Cellular Automata Model of Chlamydial Infection and Host Immune Response

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In this paper, we present a hybrid cellular automata model capable of describing the process of the ascension of infection to the upper genital tract in females and investigating the number of free chlamydial particles and infected cells. In this model, six different CA rules are introduced. On the one hand, we introduce rules to model the infection process, including how chlamydial particles enter epithelial cells, replicate and divide, based on their developmental cycle, as well as their release from spatial movement to continue the infection cycle. On the other hand, we also show the important roles of humoral and cell mediated immune cells in the clearance of free chlamydial and infected cells respectively. The motion of free chlamydial particles has been investigated by employing a diffusion partial differential equation. The qualitative results of the model reflect experimentally observed phenomena.

Tuesday 11:40–12:00 Webster 251

Quasi-Monte Carlo Methods for Derivatives on Realized Variance of an Index under the Benchmark Approach

Jan Baldeaux
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In this talk, we discuss how to apply quasi-Monte Carlo methods to the pricing of derivatives on realized variance of an index under the benchmark approach. The resulting integration problem is shown to depend on the joint density of the realized variance of the index and the terminal value of the index. We need to employ a transformation mapping this joint density to the unit cube. We establish that this transformation can be expected to determine the difficulty of the resulting integration problem. Finally, we observe that quasi-Monte Carlo methods compare favorably to Monte Carlo methods when applied to this problem.

Tuesday 4:40–5:00 Webster B

Linear Models for Endocytic Transformations from Live Cell Imaging

John Belward
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Endocytosis is the process by which cells internalise molecules such as proteins. In one form, macropinocytosis, membrane at the cell surface ruffles and folds over to give rise to an internalised vesicle. Membrane surface molecules called phosphoinositides then undergo a series of transformations that are critical for the correct trafficking of the vesicle within the cell, and which are often pirated by pathogens such as Salmonella. Advanced fluorescent video-microscopy imaging now allows the detailed observation and quantification of these events in live cells over time. Here we use these as a basis for building differential equation models of the transformations. An initial investigation of these cell interactions was modelled with reaction rates proportional to the sum of the concentrations of the individual constituents. A first order linear system for the concentrations results. The structure of the system enables analytical expressions to be obtained and the problem becomes one of determining the reaction rates which generate the observed data plots. We present results with reaction rates which capture the general behaviour of the reactions. Some excellent fits are obtained with modulated exponential functions, however these are not solutions of the linear system. The question arises as to how the model may be modified to obtain a system whose solution provides a more accurate fit.

Monday 12:20–12:40 Webster 251

Effect of Non-Negligible Wall Dielectric Constant on Electroviscous Flow

Joseph Berry, Dalton Harvie
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The steady-state, pressure-driven flow through a slit-like microfluidic contraction at low Reynolds number is investigated using a finite-volume numerical method. In this study we consider systems where the surrounding solid has a non-negligible dielectric constant, and examine the effect that this has on the development length of the electroviscous flow in the contraction. A 1:1 symmetric electrolyte liquid is considered, with a uniform charge density present on the channel walls. The effects of electric double-layer thickness and surface charge density on the flow-development length are also investigated. As the solid dielectric constant increases relative to the liquid dielectric constant, the development length of the flow increases significantly. This increase is greatest at high electric double-layer thicknesses and high surface charge densities.

Monday 4:40–5:00 Webster B

A Comparative Evaluation of Microfluidic Circuit Model Performance

Christian Biscombe
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We consider mixed pressure-driven/electro-osmotic flows through a 4:1:4 contraction-expansion microfluidic series network. We compare numerical predictions generated using two different equivalent circuit models, which are useful tools for conceptualising and designing microfluidic devices. The first, simpler approach is based on the assumption that the fully-developed average ion concentration is equal in all channels. The second, more complex approach, which was recently formulated by the authors, allows the fully-developed average ion concentration to differ between successive channels and incorporates a novel charge condition based on conservation of ion currents (rather than the total current, as in earlier models). We examine a range of experimentally relevant reservoir concentrations and surface charges and show that invoking the uniform concentration approximation can lead to substantially erroneous predictions for the pressure and potential differences across the contraction-expansion device. As expected, these errors become smaller when surface conduction effects, quantified in terms of a Dukhin number, contribute only a small fraction of the total channel conductance.

Monday 4:00–4:20 Webster B

Discrete (Riesz) Energy and Digital Nets

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Distributing (many) points uniformly in some sense over a sphere or other manifold has important applications in science and technology. Optimizing an energy functional like the classical potential energy is one way to construct configurations with good properties. The Riesz s-energy generalizes this Coulomb energy assuming point interaction based on the potential $1/r^s$ (r the Euclidean distance). The limit distribution of optimal s-energy N-point sets on a compact d-dimensional manifold is controlled by s and ranges from the usually not uniform s-equilibrium measure if $0 < s < d$ to the natural uniform measure on the manifold if $s > d$. Another question concerns the asymptotics of the optimal s-energy. Indeed, emerging from complexity theory, Problem #7 on S. Smales' list of 'Mathematical Problems for the Next Century' asks for a fast algorithm to generate nearly optimal logarithmic energy (limiting case $s \to 0$) sets which may differ at most from the optimal solution by a order of $\log N$ as $N \to \infty$. Optimal energy points are constructed using a highly non-linear optimization process. Digital Nets provide, so far, the most efficient method to generate point sets in the (high dimensional) unit cube with desirable properties like small 'discrepancy' used, e.g., for quasi-Monte Carlo rules. We investigate the discrete energy of such nets in particular on the square and lifted to the unit sphere.

Tuesday 4:20–4:40 Webster B

A Direct Method for Correcting Errors in Orthogonal Matrices Using Generalized Cayley Transforms

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A new approach to correcting errors in orthogonal matrices is presented that is faster than calculating the orthogonal polar factor. The orthogonal polar factor is known to minimize the 2-norm of the correction but the new technique often finds a correction that has a smaller maximum modulus element. The new method exploits the properties of generalized Cayley transforms that provide a characterization of the class of orthogonal matrices.

Monday 12:20–12:40 Webster 250

An Error Estimate for Krylov Subspace Approximation to the φ Function Matrix-Vector Product

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Recently, the time integration of stiff ordinary differential equations using exponential integrators has received considerable attention. The simplest example of an exponential integrator is the exponential Euler method, which is explicit in nature and offers second order accuracy in time. At the core of this method is the action of the so-called phi function of the Jacobian matrix on a suitably defined vector at each step of the integration process. The attraction of the exponential Euler method, and indeed other exponential integrator methods, is that Krylov subspace approximations to these matrix function-vector products perform well despite the absence of a preconditioner. It is noted that this is often not the case when employing Backward Differentiation Formulae (BDF) methods, where preconditioning techniques are essential to the performance of the embedded Newton-Krylov iterations. The focus of this paper concerns the task of deciding when to terminate the Krylov subspace expansion for the approximation of the phi function matrix-vector product. We propose a new a posterior error estimate and compare its performance to a well accepted estimate that is featured in the literature.

Monday 3:20–3:40 Webster 250

Projective Integration of Expensive Stochastic Processes

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Consider the case when a microscale simulator is too expensive for long time simulations necessary to determine macroscale dynamics. Projective integration uses bursts of the microscale simulator, using microscale time steps, and computes an approximation to the system over a macroscale time step by extrapolation. Projective integration has the potential to be an effective method to compute the long time dynamic behaviour of multiscale systems. However, many multiscale systems are influenced by noise. Thus it is important to consider the projective integration of such systems. By the maximum likelihood estimation, we estimate a linear stochastic differential equation from short bursts of data. The analytic solution of the linear stochastic differential equation then estimates the solution over a macroscale time step. We explore how the noise affects the projective integration in different methods. Monte Carlo simulation suggests design parameters offering stability and accuracy for the algorithms. The algorithms developed here may be applied to compute the long time dynamic behaviour of multiscale systems with noise.

Tuesday 3:00–3:20 Webster 250

Numerical Solution to the Saffman-Taylor Finger Problem with Kinetic Undercooling Regularisation

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We examine the Saffman-Taylor problem of a finger propagating in a narrow-channel Hele-Shaw cell, and find a numerical solution with the use of conformal mappings and a boundary integral method. Without any form of regularisation, there exists a one-parameter family of solutions with the width of the finger arbitrary, though in experiment only one solution with a specific finger width exists. Traditionally numerical solutions have attempted to select for the finger width by including surface tension on the interface and taking the limit that surface tension vanishes. Another option, however, is to include the effect of kinetic undercooling, relevant to ill-posed Stefan melting-freezing problems. We present the alteration of existing numerical methods to incorporate the kinetic undercooling boundary condition, and discuss the relevant solution branches.

Wednesday 10:40–11:00 Webster B

Study on Bird Flu Outbreak within a Poultry Farm with Host-Virus Model

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Bird flu or avian influenza is an epidemic disease that originates from the virulence produced by H5N1 viruses carried by wild birds. Unlike wild birds, infection of domestic birds causes serious sicknesses that eventually lead to death. In practice, spot-check is conducted to detect infection of domestic bird. If one bird in a farm is detected positive for infection, all chickens in the farm are disposed of. In this study, infection process of bird flu within a poultry farm is analyzed with a mathematical model. It is a system of differential equations for which populations of susceptible birds and infected birds and virus concentration is the unknown functions of time. A previous study shows that removal of infected birds is a crucial factor to avoid an outbreak in a poultry farm. We analyze the model further to investigate other factors to propose strategies against outbreaks of bird-flu.

Tuesday 12:20–12:40 Webster 251

Natural Convection in a Sidewall Heated Cube Using an Immersed Boundary Method

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Numerical simulation of a square cavity was conducted in order to validate an implementation of an Immersed Boundary Method (IBM). The cavity consists of two differentially heated side walls and adiabatic top and bottom walls. A Cartesian grid is used with a finite volume, fractional step pressure correction method. Simulations use Dirichlet boundaries for vertical walls and constant flux (Neumann) type boundaries for horizontal walls. The immersed boundary method involves modifying the Navier Stokes equations to include a forcing function in the momentum and energy equations that creates a virtual boundary. This method is useful because the boundary does not necessarily have to coincide with grid points, however it is much less computationally expensive than other similar methods, such as the cut cell method. The IBM is commonly used in simulations involving complex objects and can also accommodate moving boundaries. A standard numerical simulation with grid aligned with the boundary is first compared with results in the literature. The same geometry is then simulated by tilting the grid at various angles and using the IBM for each of the walls, and comparing these results with those initially obtained. This paper details the implementation method and common problems associated with this. Detailed results are presented for laminar and turbulent natural convection up to Rayleigh number 10^9.

Tuesday 11:20–11:40 Webster B

Comparison of Approximate Inverse Preconditioners for Fractional-Step Navier-Stokes Solvers

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In viscous incompressible flow simulations, fractional-step methods are applied to the Navier-Stokes equations to simplify the coupling between the pressure and velocity. This results in the sequential solution of the momentum equations and a pressure correction equation, followed by pressure and velocity updates, at each time-step. Although the pressure correction equation is solved only once in each momentum-pressure iteration, its computation uses most of the total solution time. One important characteristic of the pressure correction equation is that the coefficient matrix of the system remains constant throughout the iterations, as long as the mesh is fixed. This suggests efficiencies may be achieved by using approximate inverses as preconditioners. Approximate inverses can be constructed and stored only once, and recalled in the subsequent iterations or time-steps. An additional advantage of these methods is that their implementation in the solver requires only matrix-vector products that are relatively easy to parallelise. In this study, approximate inverse preconditioners are tested and compared to the Incomplete LU preconditioners. Both the Sparse Approximate Inverse (SPAI) and factorised Approximate Inverse (AINV) methods will be tested, amongst others. The two-dimensional time-dependent Taylor vortex problem is used as a test case, allowing the numerical solutions to be benchmarked against the analytical solution.

Monday 11:40–12:00 Webster B

Modelling of Oxygen Steelmaking

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Oxygen steelmaking is currently the dominant technology for producing steel from pig iron. The process is complex because of the presence of multiple phases (liquid metal, slag, gas, etc.), many components and the non-steady state/non-homogenous conditions within the process. Mathematical modelling has been widely used to evaluate the process and improve the process control due to the difficulties in measuring and visualizing the system at high temperatures. A computer based model has been developed that incorporates the bloated droplet theory under dynamic conditions to evaluate the influences of bloated droplet theory on the overall kinetics of the process. The basis of the theory is that when the metal droplets ejected to the slag-metal-gas emulsion, the metal droplets become bloated due to the inability of gas generated from the decarburisation reaction to escape from the surface of liquid metal droplets. The governing equations and the forms of numerical computational solution techniques for these models are explained. The model, in conjunction with the industrial data, suggests that bloated droplet theory provides a good explanation of the decarburization curves. Approximately 60% of the decarburisation takes place via metal droplets in the emulsion phase during the main blow. The advantages and limitations of these models are also critically examined and discussed.

Tuesday 3:20–3:40 Webster B

Parallel Unstructured Triangulation via Discrete Domain Decomposition

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We investigate the efficiency of a discrete domain decomposition approach to parallel unstructured triangulation for general 2D domains. We show that a balanced set of subdomains can be obtained via an initial quadtree decomposition of the full domain and that the "advancing partition" method [1] can be used to generate high quality subdomain separators. We show that these separators typically do not adversely affect the overall element quality or element distribution in the final triangulation. We obtain a parallel algorithm by allowing multiple subdomains to be meshed simultaneously via an "advancing front" approach. We also exploit the subdomain structure to achieve parallel speedups for subsequent topology improvement and smoothing phases.
[1] - Pirzadeh S and Sagaris G. "Domain Decomposition by the Advancing Partition Method for Parallel Unstructured Grid Generation." 47th AIAA Aerospace Sciences Meeting 2009; 979.

Monday 4:20–4:40 Webster 251

Tangents, Adjoints and Computational Complexity in Terrestrial Carbon Modelling

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Automatic differentiation, producing either tangents or gradients, provides a powerful way of analysing numerical models. These processes are compared by considering them firstly as algorithmic transformations, equivalent to a sparse matrix factorisation, and secondly as a vector space transformation. The vector space transformation shows how efficiencies from adjoint transformations arise due to separation of the processes of integration and differentiation. It is known that in the general case of automatic differentiation, neither the tangent nor the adjoint form will be optimal, but that the problem of finding the true optimum is NP-hard. Various aspects of modelling terrestrial carbon in earth system models are examined to identify cases where the special structure of the terrestrial model leads to useful simplifications when using automatic differentiation to analyse these systems.

Monday 4:20–4:40 Webster 250

1D Combination Technique: Its Implementation and Some Comparisons to Domain Decomposition

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The purpose of this paper is to introduce the 1D combination technique and its implementation with parallel programming. The idea of the 1D combination technique is derived from the generalised combination technique developed by Griebel, et al. (1992). In this paper, I discuss two primary features of the 1D combination technique: its reduction of computational cost, especially when combined with parallel programming and where high accuracy is required; and a resultant sacrifice of accuracy. However we will show that the loss of the accuracy can be bounded thus reducing its significance. Alternatively, by using the notions of space decomposition and subspace correction, the 1D combination technique has similarities to the parallel subspace correction method. It specifies a decomposition of the underlying finite-dimensional space, together with a way of combining the solutions of the subspaces to get a better approximation of the exact solution. I will also do some comparisons to the domain decomposition method. By using tensor products and applying the 1D combination technique in the 2D case, I illustrate that there is a possible future generalisation of this 1D combination technique to the multidimensional case. In two dimensions, this generalisation preserves the 1D combination technique's primary feature relating to cost and accuracy. Future research involves work on complexity analysis and error analysis for the multi-dimension case and comparisons with other methods.

Monday 4:40–5:00 Webster 251

A Hybrid hp-FEM - Spectral Method for the Linearised MHD Equations in Spherical Geometries

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We consider the discretisation of the magnetohydrodynamic (MHD) equations linearised about a steady basic state in spherical geometries. Poloidal-toroidal representations are used for velocity and magnetic field. The angular dependence is discretised using a Galerkin method: the basic state is expanded in vector spherical harmonics and the perturbation toroidal and poloidal potentials, and temperature are expanded in spherical harmonics. This produces a coupled system of ordinary differential equations in radius, which may contain up to fourth-order derivatives in the applications of interest, after separation of the time dependence. Previously the radial dependence has been discretised using second- and fourth-order finite differences, and Chebychev collocation. Currently we are developing a code in which the radial dependence is discretised using one-dimensional hp-finite element methods. We present investigations into aspects of one-dimensional hp-fe methods which are useful and important in the MHD applications of interest and in the implementation of the method: coupled ordinary differential equations of mixed order; multiple or higher order boundary layers; coordinate singularities; and matching conditions across material boundaries.

Tuesday 4:20–4:40 Webster 250

Estimating the Inter-Month Correlation Between Rainfall and the Atmospheric Circulation

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Inter-annual variability in the seasonal means of climate variables can arise from a number of sources which can be categorized as (a) slowly varying (inter-annual and longer) external forcing (for example, sea surface temperature forcing) and internal dynamics and (b) internal dynamics within a season. We consider that the seasonal mean of a climate variable consists of two components, referred to as the "slow" and "intraseasonal" component. A common assumption when estimating coupled patterns of "intraseasonal" variability is that the monthly statistics of the "intraseasonal" components are stationary and the underlying daily time series are first order autoregressive processes. The inter-month correlations between the pairs of climate variables are assumed to be stationary and constant. These assumptions do not hold for a variable such as rainfall where the daily data consists of dichotomous (on/off) events. It is possible to formulate a more general method for such two-state climate variables but it requires an estimate of the inter-month correlation. Here, we use a stochastic two-state first-order Markov chain model fitted to daily Australian rainfall data and daily 500hPa atmospheric geopotential height anomalies to provide such an estimate for all seasons. We show that, in general, the estimate of the inter-month correlation is much smaller than the "within-month" correlation between rainfall and the 500hPa height "intraseasonal" component.

Monday 10:40–11:00 Webster 251

Role of Dynamical Modes in Changing Southern Memisphere Climate

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Krylov subspace and direct methods are compared for generating the leading dynamical normal modes of large systems of differential equations describing atmospheric flows. The methods are applied to examine the roles of leading eigenvectors in describing the changing Southern Hemisphere weather transients during the the 20th century. During the last sixty years there have been large changes in Southern Hemisphere winter circulation and reductions in rainfall particularly in the southern Australian region. Here we examine the corresponding changes in leading dynamical eigenmodes of variability that we show may be related to important weather transients. Our study is performed using a global two-level primitive equation instability-model with reanalyzed observed July three-dimensional basic states for the periods 1949-1968, 1975-1994 and 1997-2006. We relate the reduction in the winter rainfall in the Southwest of Western Australia (SWWA) since the mid-1970s and in Southeastern Australia since the mid-1990s to changes in growth rate and structures of leading storm track and blocking modes. We find that cyclogenesis and onset of blocking modes growing on the subtropical jet have significantly reduced growth rates in the latter periods. On the other hand there is a significant increase in the growth rate of Northwest cloud-band modes and intraseasonal oscillations disturbances that cross Australia and some smaller increase in the intensity of African easterly waves.

Monday 10:40–11:00 Webster B

Estimating Components of Covariance Between Two Climate Variables Using Model Ensembles

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The seasonal mean variability of a climate variable can be considered as components relating to three sources: (a) slowly varying external forcings on time scales longer than a season (eg, radiative forcing, response to sea surface temperature), (b) slowly varying internal (atmospheric) forcings, and (c) internal forcings on time scales of less than a season. Using an Analysis of Variance-based method, the interannual variability of the seasonal mean of a climate variable from a coupled atmosphere-ocean general circulation model ensemble can be separated into these slow-external, slow-internal and intraseasonal components. However, to understand the nature of these modes of variability, their relationship to other climate variables must be examined. Here, we extend the method of separation of components of variability to the covariance between projected time series of the modes of variability and a climate variable representing a possible source of variability. To illustrate this, we estimate the interannual modes of variability of monthly mean 500hPa geopotential height from ensembles of coupled model realisations. The components of covariance are then obtained between the projected time series of these modes and the ensemble sea surface temperature. We show that the nature of the slow-external and slow-internal modes is more clearly understood than by using time series correlations.

Monday 10:20–10:40 Webster 251

An Implicit Finite Volume Method for Arbitrary Transport Equations

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A new finite volume algorithm (‘arb’) is described that can be applied to a variety of heat, mass and momentum transport problems. The algorithm is constructed in a unique way: The transport equations and associated boundary conditions are input by the user using pseudo-mathematical expressions. A perl program then reads these equations, and via the symbolic algebra package ‘maxima’, ‘metaprograms’ fortran source code that solves the problem using a multidimensional Newton-Raphson method on an unstructured mesh. The strength of the technique is that a fully implicit numerical formulation can be generated and modified easily, for any arbitrary set of transport equations. Within this talk the data structures and programming techniques employed in the technique are detailed, and the resulting algorithm’s performance when solving representative heat diffusion and fluid dynamics problems is discussed. The algorithm is freely available under the Gnu General Public License (GNU GPL).

Monday 12:20–12:40 Webster B

Study of River Flow Based on Finite Element Analysis and GPS-Echo-Sounder Measurement

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Mathematical techniques are applied to analyze problems in water environment. In this work currents of a river are analyzed numerically by introducing data concerning the water depth into finite element analysis of partial differential equations of flow. Techniques to simulate currents generated in a river are described. A region is divided in the vertical direction into layers, and a finite element discretization in the horizontal direction is applied. Results of simulation of flow generated in Yoshii River in Okayama Prefecture of Japan will be introduced. We also introduce our techniques to measure the river bed topography using a hardware system consisting of a global positioning system (GPS) and an echo sounder. Data obtained by using the system are introduced into analysis of flow and numerical results will be introduced.

Wednesday 10:40–11:00 Webster 250

A Parametric Investigation of Natural Ventilation Flow with a Line Heat Source

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The effects of Reynolds number (Re) and Prandtl number (Pr) on natural ventilation flow with a line heat source were investigated using two-dimensional numerical simulations. Four different scenarios were considered: varied Re with a fixed Pr at 7, varied Pr with a fixed Re at 500000, varied Re and Pr with a fixed Rayleigh number ($Ra=Re^2*Pr$) at $1.75*10^{12}$ and varied Re and Pr with a fixed heating rate (Re^2/Pr). Opposite effects on turbulent characteristics such as frequency and spectral amplitudes were observed for increasing Re and increasing Pr. The start-up flow for natural ventilation, consisting of a semi-confined plume, was also investigated, and relationships for initial start-up velocity and time taken for onset of a turbulent mode were found as a function of Re.

Tuesday 10:00–10:20 Webster B

Simulation of Multiple Obstacle Acoustic Scattering in Three Dimensions

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We describe an efficient algorithm for simulating low to medium frequency acoustic waves scattered by ensembles of tens or even hundreds of three dimensional particles. A key component of our surface integral algorithm is the high-order approximation of the surface field on each particle in the ensemble. The high-order approximation leads to linear systems with a block structure in which each block has considerably smaller dimension than would be obtained using low-order boundary element methods. For many problems at low to medium frequency, the dimension is sufficiently small that single scattering problems can be quickly solved using LU factorisation. This property allows rapid solution of the multiple scattering problems using iterative solution methods based on fast solution of single scattering problems on each particle and fast evaluation of induced fields on the other particles. We demonstrate the algorithm through simulation of acoustic interactions in ensembles consisting of tens or hundreds of particles.

Monday 11:40–12:00 Webster 250

Using Matlab to Summarise Sea Temperature and Wind Data in a Survival Analysis of Little Penguins

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Sea-surface temperature and wind data from January 1967 to December 2008 (provided by the Bureau of Meteorology, Melbourne) are used as covariates in a statistical analysis. The sea-surface temperature data have a 1° by 1° resolution, with the grid of sea-surface temperature values running from 138° East to 152° East and from 35° South to 45° South. For each month, there are 10 rows and 14 columns of data corresponding to the monthly mean sea surface temperature at the mid-point of each grid square. Wind data from Laverton RAAF Base, Victoria are given as magnitude and direction readings at 9.00 am and 3.00 pm each day. We use Matlab to summarise sea-surface temperature and wind data, and to conduct a mark-recapture analysis. We illustrate our methods by investigating the effect of local westerly winds and sea-surface temperature on the survival of Little Penguins on Phillip Island, Victoria using data from a 42 year study.

Tuesday 5:00–5:20 Webster 251

On the Numerical Solution of the Chemical Master Equation with Sums of Rank One Tensors

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We show that sums of rank one tensors (or separable functions) representing the so-called CP-decomposition can be used effectively to solve the chemical master equations as in many cases the effective tensor (CP) rank of the probability distribution only grows slowly with time. Both theoretical bounds and computational experiments are presented which support this claim. The proposed numerical algorithm is thought to provide an effective tool for the computational study of stochastic biochemical systems involving large numbers of different chemical species.

Tuesday 10:20–10:40 Webster 251

Controlled Drug Release from Polymeric Spheres

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In the pharmaceutical industry, the development process of a new drug can be facilitated enormously by mathematical modelling of drug release mechanisms, which directly decreases the number of necessary experiments. One particular controlled drug release mechanism based on the polymer's physiochemical properties is swelling. A mathematical model for this type of mechanism leads to a moving boundary problem for both the concentration of solvent in the polymer substrate and the concentration of drug in question, with the swelling domain enclosed by two moving boundaries. We explore this model numerically and analytically; the results are discussed and comparisons are made with the literature.

Wednesday 10:40–11:00 Webster 251

Applications of CFD Modelling in Metallurgical Process Industries

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With the advancement of high performance computing facilities, CFD modelling technique has evolved as a powerful tool for the researchers working in the metallurgical field. CFD can predict flows ranging from simple single phase flows to complex multiphase flows in high temperature combusting environment associated with metallurgical process industries. Successful and efficient development of a CFD model can predict the fluid flow behaviour, combustion behaviour, generation of turbulence and splashing and other fluid dynamic parameters inside the furnace. Present authors have developed a CFD model for zinc slag fuming process for top submerged lance smelting furnace. The model integrates complex combustion phenomena and chemical reactions with the heat, mass and momentum interfacial interaction between the phases present in the system. The model is based on 3-D Eulerian multiphase flow approach and it predicted the velocity and temperature field of the molten slag bath, generated turbulence, vortex and plume shape at the lance tip. The model confirmed that rate of zinc fuming increases with temperature and is broadly consistent with experimental data. Though the model is based on zinc slag fuming for top submerged lance injection case, it can be expanded or applied to any other smelting process. This model is a significant step in developing comprehensive model for metallurgical process industries.

Tuesday 3:00–3:20 Webster B

Weighted K-Word Matches: a Sequence Comparison Tool for Proteins

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A common problem faced by biologists is to find closely related DNA or protein sequences. Sequences with a high degree of similarity are believed to be closely related in terms of evolutionary distance or to have evolved to perform functionally similar tasks. Fast algorithms are needed to search large databases to find close matches to given query sequences. The most commonly used algorithm (BLAST) searches for and attaches significance scores to long alignments. BLAST generally performs well, but fails when long-range contiguity has been compromised by shuffling, duplication, deletion or inversion of extended blocks of sequence. An alternate alignment-free method is to use k-word matches, in which a significance score is attached to the number of exact matches of short words of pre-specified length k. The algorithm is extremely fast, performing at least as well as BLAST for simulated evolutionary DNA sequences. Here we extend the algorithm to amino-acid sequences. A weighted word match count is defined which reflects the varying degrees of similarity between pairs of amino acids. We have computed and simulated the mean, variance, and distribution function for various forms of the weighted word match statistic for sequences of identically and independently distributed letters. We present these results and a method for choosing an optimal word size. The efficiency of the method is tested by using simulated evolutionary sequences, and the results compared with BLAST.

Monday 12:00–12:20 Webster 251

Finite Element Modelling of Insertion of Electrode Array into the Cochlea with Lubricant

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The cochlear implants consisting of electrode arrays for electrically stimulating the auditory nerve fibres have been developed to restore hearing for profoundly deaf people. The insertion of a straight electrode array into the spiral cochlear scala tympani has unfortunately been found to damage delicate structures within the inner ear such as the spiral ligament and the basilar membrane. Although a number of studies suggested the use of lubricant for smooth insertion, little attempt has been made to quantitatively study the effect of lubricant on the damage by the electrode array to the cochlear structures. In this study, a mathematical model using the finite element method was developed to predict the trajectories of the Nucleus standard straight electrode array during insertion into the scala tympani and associated contact stresses exerted by the array on the cochlear structures. Results from the model have shown that the use of a lubricant such as glycerine reduces the contact stresses exerted by the tip of the array on the spiral ligament from 0.3 to 0.2 MPa, whereas the contact stresses on the basilar membrane reduce from 0.075 MPa (without lubricant) to 0.025 MPa (with lubricant). The results suggest that the use of a lubricant is clinically important for minimising the likelihood of damage by the electrode array to the cochlear structures.

Tuesday 3:20–3:40 Webster 251

A Numerical Investigation of the Thermal Performance of a Solar Chimney

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This paper reports a numerical study of the air flow inside a solar chimney in order to predict its thermal performance in terms of ventilation rate and heat transfer. Both convection and radiation heat transfer are considered as the mechanisms through which thermal energy is transferred into the air. A steady-state two dimensional solar chimney model is considered with more realistic thermal boundary conditions: adiabatic and iso-flux. The conservation and transport equations that describe the flow and heat transfer in the solar chimney are solved using a finite volume technique. Numerical results will be derived for a solar chimney with absorber height 1.5 m and different air gap widths. The study will focus on the effects of the Rayleigh number and aspect ratio as well as radiation effect on the thermal performance of the solar chimney and also various heat fluxes will be considered in order to show the effect of input heat on ventilation performance. Detailed results obtained from the numerical simulation will be presented and discussed.

Monday 4:20–4:40 Webster B

Subgrid Parameterisations for High Resolution Atmospheric Flows

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Numerical and computational methods are presented for the Large Eddy Simulation (LES) of quasi-geostrophic atmospheric flows on a sphere. The flow fields are generated using a spectral code written in spherical coordinates. Simulations are undertaken for a wide range of truncation wavenumbers to determine the influence of resolution on the LES subgrid parameterisations. A stochastic model is used to represent the subgrid scales of motion by a drain viscosity and a stochastic backscatter term. Two LES variants are presented: an isotropic parameterisation, in which the model coefficients are only a function of the total wavenumbers; and an anisotropic parameterisation, that is dependent on both the zonal and total wavenumbers. For both schemes, the subgrid coefficients are derived from a high resolution reference Direct Numerical Simulation (DNS) data set. The reference DNS has 504 zonal and total wavenumbers. This is equivalent to 1436 longitudinal and 768 latitudinal grid points, or a grid point approximately every 0.25 degrees. Both LES variants are shown to replicate the energy spectra of the DNS data set. The effect of the truncation wavenumber on the subgrid viscosity and backscatter terms is also investigated, and a self-similar scaling of the subgrid coefficients is sought. A universal scaling of these coefficients would enable the present approach to be applied to more general cases.

Monday 3:00–3:20 Webster B

Irrelevance of the Fractal Term in the Fractal Attrition Equation

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The Fractal Attrition Equation (FAE) models the casualties predicted by Map Aware Non-uniform Automata (MANA), an agent based combat modelling distillation, at each MANA timestep. The FAE has three important differences from the simple early 20th century models of casualties that used only the numbers on each side to make predictions. Firstly, only those agents within range of the enemy may inflict casualties. Secondly, the detection range is assumed to be greater than the range of weapons and a fitting factor, c, assumed to represent the effect of the gap between these two ranges, is introduced. This builds in one of the assumptions of Network Centric Warfare (NCW), that you will be able to see your enemies before they can shoot at you. Thirdly, and novelly, a fractal dimension is introduced. We postulate that the important part of the information used in calculating the fractal dimension has already been incorporated into the model through the consideration of range. We test this hypothesis by comparing the outcomes of the FAE and the FAE without the fractal term on three scenarios: that used by the developers of the FAE; best practice MANA tactics from the literature; and a rout scenario. The results show no significant difference in fit to the MANA data between the two models and we conclude that the fractal term in the FAE is redundant.

Monday 5:00–5:20 Webster 250

A New Stopping Rule of the GMRES Method for Linear Discrete Ill-Posed Problems

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The Fredholm integral equation of the first kind is one of models derived from inverse problems. After discretisation of the equation, severely ill-conditioned linear system is generated. We will propose a new stopping criterion and modification of the GMRES method for solving the linear discrete ill-posed problem. Recently, Krylov subspace methods are popular for the problem as regularization methods. However, the ill-conditioned system is too sensitive to measurement errors to obtain an appropriate approximate solution by only solving it with the classical Krylov subspace methods. Then, modification of the methods and decision of the approximate solution are important. In particular, focusing on the GMRES method, we will propose a new stopping rule using an idea of Tikhonov regularization and a modified GMRES method with it.

Tuesday 12:20–12:40 Webster 250

Numerical Solution of a Parabolic Equation on the Sphere Using Laplace Transforms and RBFs

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We propose a method to construct numerical solutions of parabolic equations on the unit sphere. The time discretisation uses Laplace transforms and quadrature. The spatial approximation of the solution employs radial basis functions (RBFs) restricted to the sphere. The method allows us to construct high accuracy numerical solutions in parallel.

Tuesday 4:40–5:00 Webster 250

Numerical Solutions of the Stokes Equations on the Unit Sphere By Radial Basis Functions

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Constructing efficient algorithms to simulate Stokes and Navier-Stokes equations (NSEs) on spherical surfaces plays a major role in many climate models on the global scale. Spherical radial basis functions (SRBFs) present a simple and effective way to construct numerical solutions for partial differential equations on smooth surfaces, compared to mesh based methods. The SRBFs based methods are meshless and implementation of such methods is simple, thanks to efficient choices of SRBFs on domains and surfaces. In this paper, as a stepping stone towards developing an efficient SRBF algorithm for the full NSEs, we propose and analyse a meshless method for the Stokes equations on the unit sphere using divergence-free SRBFs.

Monday 12:00–12:20 Webster 250

Preconditioners for Interpolation of Surface Divergence-Free Vector Fields on Spheres

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Surface divergence-free RBFs based on scattered data are introduced recently by Narcowich, Ward and Wright to interpolate divergence-free vector fields on surfaces. The linear system arising from this interpolation problem tends to be ill-conditioned when the separation radius of the scattered data is small. When the surface under consideration is the unit sphere, we introduce a preconditioner based on the additive Schwarz method to accelerate the solution process. Theoretical estimates for the condition number of the preconditioned matrix will be given. Numerical experiments using scattered data from MAGSAT satellite show the effectiveness of our preconditioner.

Tuesday 11:40–12:00 Webster 250

Rates of Convergence of Quadratures for Weighted Tensor Product Spaces on the Torus

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In [1], Hesse, Kuo and Sloan describe a component-by-component method for quadrature on weighted tensor product spaces (WTP) defined on products of unit spheres. We examine the equivalent method in the more familiar setting of WTP spaces on the torus, and compare it with a version of the sparse grid quadrature algorithm of Wasilkowski and Wozniakowski [2] adapted to this setting. In particular, we compare the initial and asymptotic convergence rates of the two methods, giving both theoretical bounds and numerical results for each, for different rates of decay of the dimension weights.
[1] K. Hesse, F. Y. Kuo and I. H. Sloan, A component-by-component approach to efficient numerical integration over products of spheres. Journal of Complexity,23(1), 2007, pp.25- 51.
[2] G. W. Wasilkowski and H. Wozniakowski, Weighted Tensor Product Algorithms for Linear Multivariate Problems. Journal of Complexity, 15(3), 1999, pp. 402-447.

Tuesday 5:00–5:20 Webster B

3-D Hydrodynamics in Darwin Harbour, Northern Territory

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This research principally aims to build a 2-D and 3-D hydrodynamic model for Darwin Harbour based on RMA (Resource Management Associates/Association) model. RMA is a series of finite element hydrodynamics and water quality model capable of simulating one-, two-, or three-dimensional coastal waters, such as estuaries, bays, lakes, and rivers. Variables that are included in the model are temperature, salinity, current velocities, nutrients, and suspended sediment concentration. The finite element method with quadratic approximation is used to solve these equations. The model bathymetry data includes the high resolution Darwin Harbour coastal line, sea surface area and mangroves distribution with a minimum grid cell of 50 m. The model will be forced by tides at the open boundary. The observed sea surface height data (SSH) from June 17th in 2009 were used to calibrate the model. The model simulation shows that near East Arm of Port Darwin, the tides are dominantly semi-diurnal and the largest tidal range can reach 8 m and the main tidal constituents are M2, K1, S2, and O1. M2 is the largest tidal constituent with amplitude 1.99 m and phase 189 degrees. At spring tides, the peak flood currents velocity is more than 1 m/s which occurred near the East Arm, and is slightly bigger than the peak ebb currents. The 3-D RMA model has been implemented and model validation/calibration is currently in progress.

Monday 10:00–10:20 Webster B

Parameter Estimation for a Phenomenological Model of the Cardiac Action Potential

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The cardiac action potential (AP) is made up of a complex balance of ionic currents which flow across the cell membrane in response to electrical excitation of the cell. Mathematical models of the action potential have grown increasingly complex, featuring as many as 67 variables. The fitting of parameters to large models such as this has increasingly seen a large degree of parameter and module re-use from earlier models, which may be inconsistent in factors such as species or the temperature of experiment. An alternative method for modelling cardiac tissue is a phenomenological model, which seeks to reconstruct the behaviour of the AP without resorting to the use of a biophysically detailed model. Properties such as AP morphology, dynamic restitution and conduction velocity restitution may all be fitted using this approach. In this paper, we use some techniques for parameter estimation to fit the morphology of the AP in the four variable Bueno-Orovio phenomenological model. A modified hybrid Nelder-Mead simplex search and particle swarm optimization to turn the parameter estimation problem into a minimisation problem. We use both data generated from the Luo-Rudy I model of a guinea pig ventricular myocyte and also experimental AP traces. The method is capable of accurate reproduction with the model of both experimental and model generated APs, showing its ability to fit a complex morphology to a model with substantially more parameters than previously demonstrated.

Wednesday 10:20–10:40 Webster 251

Determining Critical Conditions for 2D Compost Piles with Air Flow via Numerical Simulations

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We consider the self-heating process of a 2D spatially dependent model of a compost pile. This model incorporates terms that account for self-heating due to both biological and oxidative mechanisms. The self-heating model consists of mass balance equations for oxygen and energy. We study the effects of air flow through the pile. We utilize numerical solutions to determine critical conditions for thermal ignition within the compost pile. Once confronted with a numerical means to solve a problem, it is necessary to be a little circumspect about the results and seek an independent means to corroborate them. For this reason, the present paper uses two distinct numerical approaches to determine the solutions to self-heating problem in compost piles. Firstly, we analyse the model numerically by using the FlexPDETM (a commercial software package) in a 2D configuration. FlexPDETM is a space and time adaptive finite element package, and therefore both time and space errors can be minimized. The results obtained by using FLEXPDETM were then compared with those obtained using the method of lines (MOL) in which the governing partial differential equations (PDEs) and boundary conditions are transformed into a system of ordinary differential equations (ODEs) using finite differences. We then utilize MATLABs ODE solver routines to solve the system of ODEs. We focus mainly on the critical conditions for thermal ignition for different rates of airflow moving through the compost pile.

Monday 10:00–10:20 Webster 250

Wavelet Based Solution to Solve Flow and Diffusion Problems in Digital Materials

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Tomographic imaging can now be routinely performed over three orders of magnitude in length scale with correspondingly high data fidelity. This capability, coupled with the development of advanced computational algorithms for image interpretation, three-dimensional visualization, structural characterization and computation of physical properties on image data, allows for a new numerical laboratory approach to the study of real complex materials: the Digital Materials Laboratory. The computation of physical properties in a digital materials laboratory requires significant computational resources. For large 3D data sets, the number of data points is of the order of 8 billion; even for a simple binary image, we can benefit from a more efficient numerical approach to solve the problem. Due to the complex nature of the media, one of the most difficult problems to solve is the multiphase flow problem, and traditional methods such as Lattice Boltzmann are not attractive as the computational demand for the solution is too high. A wavelet-based algorithm reduces the amount of information required for computation. Here we solve the Poisson equation for a large 3D data set with a second order finite difference approximation. Constraints and fictitious domains capture the complex geometry. We solve the discrete system using the discrete wavelet transform and thresholding. We show that this method is substantially faster than the original approach and has the same order of accuracy.

Tuesday 3:00–3:20 Webster 251

Computational Approaches to Modelling Chlamydia Infection

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Chlamydia, the most common sexually transmitted bacterial infection in humans, is an interesting infection for mathematical modellers. On the micro scale, it exhibits a unique and relatively complex biphasic developmental cycle, while on the macro scale it tends to reach a dormant, asymptomatic and persistent state leading to serious genital and ocular health conditions making Chlamydia the most costly sexually transmitted infection other than HIV/AIDS. In this paper we discuss the computational approaches currently employed for modelling Chlamydial infection at various scales.

Tuesday 11:20–11:40 Webster 251

Modelling of Phosphine Distribution in Vertical Grain Storage

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Fumigation by phosphine is a common method for killing insects in grain storage to preserve the quality standard requirements for grain export. The phosphine will only be effective if the concentration is sufficiently high in all parts of a grain silo and if insects are exposed to phosphine for a sufficient time. An axisymmetric fumigant transport model has been developed to study the concentration distribution in a vertical grain storage over time. The model is a 3-dimensional advection-diffusion transport model with a sink term for the sorption of phosphine into the grain. The governing equations are solved numerically using a software package, COMSOL, which is based on a finite element method. Findings from this work for a vertical grain storage suggest that the top part of the grain is not receiving a sufficient dosage. This suggests creating a more effective fumigation design that will eventually lead to a successful fumigation.

Monday 10:20–10:40 Webster 250

Environmental-Based Production Planning Problem of Crude Palm Oil Industry under Uncertainty

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Industry plays an important role in economic development for a country and could enhance the economic welfare of its people. However, the process taken place in industry causes damage to the environment and human health. For the crude palm oil industry despite obvious benefits could be obtained from this industrial sector, it contributes to environmental degradation from both input and output sides of its activities. On the input side, crude palm oil mill uses much water in production process and consumes high energy. On the output side, manufacturing process generates large quantity of wastewater, solid waste/by-product and air pollution. In environmental production planning and risk management decision process in crude palm oil industry, there are several alternatives need to be analyzed in terms of multiple noncommensurate criteria, and many different stakeholders with conflicting preferences are involved. The inherent uncertainty of data (e.g. demand, price), together with the sequential evolution of data over time leads the production planning problem to a mixed-integer stochastic programming model. We use scenario generation based approach and feasible neighborhood search for solving the model. Keywords : Crude-Palm oil, Environmental Production Planning, Stochastic Programming, Modeling, Recycling

Monday 3:00–3:20 Webster 251

Heterogeneous Computing and the Finite Volume Method for Simulation of Flow Through Porous Media

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Heterogeneous computing, utilising high-speed graphics processing units (GPUs) along with multi-core central processing units (CPUs) to accelerate computationally intensive tasks, is an exciting recent development with direct application to computational mathematics. However, for many practical problems, it is currently very challenging to write software to fully utilise such hardware. We present a finite volume method for simulation of flow through porous media. Unstructured meshes and heterogeneities in material properties give rise to irregular memory usage and data processing patterns, which do not map directly onto the data-parallel GPU architecture. We show how basic operations such as interpolation and gather-scatter can be described in terms of data-parallel operations that can be optimised on both CPUs and GPUs. Compile-time dispatching with C++ templates is used to facilitate different implementations of basic operations on vector data, with an appropriate processor (CPU or GPU) selected depending on whether the data resides in host or device memory. Multi-core CPUs are supported through the widely-used parallel application programming interfaces (APIs) OpenMP and MPI, while NVIDIA's CUDA API is used to write GPU-accelerated operations. With this approach, only the basic operations need to be rewritten for new environments, and users developing models will call these operations, minimising the need to explicitly write code for specific hardware configurations.

Monday 4:00–4:20 Webster 251

Model Selection Procedures for High-Dimensional Genomic Data

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Many complex diseases are thought to be caused by multiple genetic variants. Recent advances in genotyping technology have allowed investigators of a complex disease to obtain data for a massive number of candidate genetic variants. Typically each candidate variant is tested individually for an association with the disease. We approach the problem as one of model selection for high-dimensional data. We propose a method whereby penalised maximum likelihood estimation is used to provide a reasonably sized set of variants for inclusion in our model. We then perform stepwise regression on this set of variants to arrive at our model. Penalised maximum likelihood estimation is performed with both the lasso and a more recently developed method known as the hyperlasso, with smoothing parameters chosen by cross-validation. The hyperlasso has a penalty function that favours sparser solutions but with less shrinkage of those variables that are included in the model, when compared to the lasso, however this comes at extra computational cost. We apply the above method to a large genomic data set and use resample model averaging to assess model performance. In particular we investigate model stability, the effect of multicollinearity, and computational cost.

Monday 11:20–11:40 Webster 251

Numerical Entropy Production for Shallow Water Flows

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We propose a numerical scheme of the entropy for the one-dimensional shallow water wave equations. The numerical scheme follows from a well-balanced finite volume scheme of the quantity vector having water height and momentum as its components. The local truncation error of the entropy is called the numerical entropy production, and can be used to detect the location of a shock discontinuity. We show by numerical tests that the numerical entropy production performs better in detecting such discontinuity than some local truncation errors of the quantity.

Monday 12:00–12:20 Webster B

A New Analytical Solution for Testing Debris Avalanche Numerical Models

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An analytical solution to a debris avalanche problem in the one-dimensional topography-linked coordinate system has been found by Mangeney, Heinrich, and Roche [Analytical solution for testing debris avalanche numerical models, *Pure and Applied Geophysics*, 157:1081-1096, 2000]. In this article, we extend the presentation of Mangeney et al. We derive an analytical solution to a debris avalanche problem in the standard Cartesian coordinate system. A characteristic method and a transformation technique are used to obtain the analytical solution. This analytical solution is used to test finite volume methods with reconstruction of the conserved quantities based on: either stage, height, and velocity; or stage, height, and momentum. The numerical tests show that the finite volume method with reconstruction based on stage, height, and momentum is more accurate in solving the debris avalanche problem.

Wednesday 10:00–10:20 Webster B

Modeling Coordination Relationship in School Communities Using Markov-Based Dynamic Influence Diagram

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The world today concerns with environmental problems, such as, global warming and climate change. Most of the environmental problems might be caused by human behavior.The most effective way to enhance environmental behavior is through education. The communities involved in the educational system of a school can be regarded as a multi agent system. It is well known that the necessity of managing relationships among agents in multi-agent system is to achieve coordinated behavior. One approach to manage such relationships consists of using an explicit representation of them, allowing each agent to choose its actions based on them. In the educational system each agent is allowed to choose its action based on them. In this paper we address an approach to represent coordination relationships assuming that agents inhabit an uncertain condition. We use Markov-based dynamic influence diagram to model the coordination relationships such that agents are able to both represent and infer how their activities affect other agents activities in a way to achieve the environmental behavior objective. Keywords : Education, Environmental Awareness, Influence diagram, Markov Process, Multi-Agent System

Tuesday 10:00–10:20 Webster 251

Constructing Positive Definite Circulant Embeddings in Higher Dimensions

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Circulant embedding is an accurate and efficient way to generate realisations of a stationary Gaussian random process with specified covariance function via a single FFT of shaped white noise. It requires, however, that the simple periodic extension of the covariance function is itself positive definite. In one dimension this holds in most cases; in higher dimensions, unfortunately, the straightforward extension often fails to be positive definite. This paper shows, however, that a more careful construction yields positive definite extensions in such situations. The paper is motivated by the result in Wood (1995) and Dietrich & Newsam (1997) that in one dimension the simple periodic extension is positive definite if the covariance function is convex and decreasing. The paper generalises this to higher dimensions: if a closed contour exists within which the covariance function's Laplacian is positive and along which its outward pointing normal derivative is negative then the function has a positive definite periodic extension. This constructed by enclosing the contour in a hypercube, clipping the function within the hypercube but outside the contour to its value on the contour, and reflecting across the hypercubes boundaries. The result has theoretical and practical applications: it can be used to construct random fractals whose covariance functions truly are power laws and to generate simulations whose statistics better match empirically estimated covariances.

Tuesday 4:00–4:20 Webster B

Circulant Embeddings for Toeplitz Covariance Matrices

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Gaussian random fields on uniform rectangular grids, with isotropic covariances, are characterised by block-Toeplitz (with Toeplitz blocks) covariance matrices. When producing instances of the random field, it is efficient to embed the covariance matrix in a block circulant matrix, and apply Fourier methods to find the eigenvalue decomposition. We present results demonstrating that integrations over the embeded probability space remain consistent with the original probability space, and minimal requirements of the embedding to ensure positive definiteness of the circulant matrix.

Monday 4:00–4:20 Webster 250

An Ensemble Prediction Study of the East Australian Current

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We present an ensemble prediction study (EPS) of the East Australian Current (EAC) with a specific focus on the examination of the role of dynamical instabilities and flow dependent errors of the day. The region where the EAC separates from the coast, is characterised by significant mesoscale eddy variability, meandering and is dominated by non-linear dynamics thereby representing a severe challenge for operational forecasting. Using analyses from the Australian operational ocean forecast system (OceanMAPS) we explore the structures of flow dependent forecast errors over 7 days and examine the role of dynamical instabilities. Forecast ensemble perturbations are generated using the method of bred vectors allowing the identification of those perturbations to a given initial state that grow most rapidly. We consider a 6 month period spanning the Australian summer beginning in mid November through to mid May that corresponds to the period of maximum eddy variability. We find that the bred vector (BV) structures align and anti-correlate with the forecast errors (see figure 1) and that these structures typically occur in regions of instability and in particular where the EAC boundary current separates. We also find that very few BVs are required to identify regions of large forecast error and on that basis we expect that even a small BV ensemble would prove useful for adaptive sampling and targeted observations.

Monday 3:20–3:40 Webster B

Reconstruction with Blobby Shapes

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This paper investigates fitting a surface to an object using blobby models as a coarse level approximation. The aim is to achieve a given quality of approximation with relatively few parameters. This process involves an optimization procedure where a number of blobs (ellipses or ellipsoids) are separately fitted to a cloud of points. Then the optimized blobs are combined to yield an implicit surface approximating the cloud of points. The results for our test cases in 2 and 3 dimensions are very encouraging. For many applications, the coarse level blobby model itself will be sufficient. For example adding texture on top of the blobby surface will give a surprisingly realistic image. For other problems finer detail will be needed. Such detail can be added by using the blobby model as the coarsest level of a hierarchical model, with radial basis function approximations used refine the implicit surface at the finer levels.

Tuesday 4:20–4:40 Webster 251

Numerical Study on Effects of Tsunami Based on Finite Element Method

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Effects of tsunamis generated in water areas surrounding Japan are studied numerically. Partial differential equations consisting of momentum equations and a continuity equation are reduced to a system of ordinary differential equations with discretization based on a finite element mesh, and a ODE solver is applied to the resultant system to generate numerical solutions. Depth data formulated in terms of longitude and latitude in horizontal direction are transformed to generate input data in terms of projected coordinates by the Gauss-Krüger projection. Numerical results are visualized, and effects of tsunami such as wave heights, propagation speeds, and run-ups are illustrated. Numerical techniques to simulate tsunamis will be described, and numerical results will be introduced.

Wednesday 10:20–10:40 Webster 250

A Bioinformatic Application of Mutual Information Between Discrete and Continuous Variables

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Experimental work in genetics creates large quantities of high-dimensional data. The systems biology approach attempts to integrate these multiple sources data: including gene expression levels, single nucleotide polymorphisms (SNPs) and clinically measured phenotypic outcomes. A natural way to express the relationship between these data is via a network of associations, such as a correlation matrix. Information theoretic and machine learning techniques such as mutual information (MI) and clustering can be used to identify properties of these networks. We extend a previous approach (Zhang & Horvath, 2005) by using MI as a measure of association that is valid for both continuous and discrete variables. If the continuous distribution is represented as a mixture of distributions for each level of the categorical variable, the MI between a continuous and discrete variable can be shown to be a weighted sum of Kullback-Leibler divergences for each category. Estimation is made computationally tractable by using a well known FFT-based kernel density estimate (Wand & Jones, 1995) which gives estimated values for the continuous density function on a regularly spaced grid of points. The use of a Gaussian kernel results in smooth density estimates that allow the Kullback-Leibler divergences to be easily integrated by Simpson's rule. This is implemented in R with computational bottlenecks identified and sped up through compiled linked libraries written in C.

Monday 10:00–10:20 Webster 251

An Additive Schwarz Preconditioner for Pseudodifferential Equations Using Spherical Splines

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We present an overlapping domain decomposition technique for solving the Laplace-Beltrami equation and the hypersingular integral equation on the sphere with spherical splines. We prove that the condition numbers of the additive Schwarz operators are bounded by $O(H^2/h^2)$ and $O(H/h)$ respectively, where H and h are the sizes of the coarse and fine meshes. Better bounds of $O(H/\delta))$ and $O(\log^2 H/\delta)$ for these two equations respectively are presented in the case the degree of splines is even. Here J is the number of subdomains, δ is the size of the overlap. Some numerical experiments which use data from MAGSAT satellite will be presented to illustrate our theoretical results.

Tuesday 11:20–11:40 Webster 250

Applications of l_1 Regularisation

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The lasso algorithm imposes an l_1 norm bound constraint on the variables in least squares models and then tunes the model estimation calculation using this bound. This leads to a form of quadratic program which can be solved by a straight-forward modification of an active set algorithm for each value of this bound. Considerable interest was generated by the discovery that the complete solution trajectory parametrised by this bound can be calculated very efficiently. Essentially it takes no more work than the solution of either the unconstrained least squares problem or the quadratic program for a single bound value. This has resulted in the study both of the selection problem for different objective and constraint choices and of applications to such areas as data compression and the generation of sparse solutions of very under-determined systems. One class of generalisation is to estimation problems with piecewise linear objective functions. Our original continuation idea extends to these polyhedral objectives in an interesting two phase procedure which switches between the constrained and Lagrangian forms of the problem. However, it is significantly less computationally effective than is the original algorithm for least squares objectives. In contrast, a relatively efficient descent algorithm is available for fixed values of the constraint bound.

Tuesday 10:00–10:20 Webster 250

Solving Variational Inequalities Using Adaptive Wavelet Methods

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We consider constrained minimisation problems of the form $\inf_K F$ where K is a convex set in a Hilbert space V and $F : V \to \mathbb{R}$ is a differentiable function. By using a Riesz basis in V we recast the problem in the sequence space ℓ_2, design a projected gradient algorithm, and study its properties. We use wavelets to recast elliptic variational inequalities as constrained quadratic optimisation problems in ℓ_2 which are solved with the projected gradient algorithm. The so obtained method is then analysed further. Finally we present numerical examples and discuss applications to obstacle problems, stochastic games, and pricing American options in high dimensions.

Wednesday 10:00–10:20 Webster 250

A Well Balanced Scheme for the Shallow Water Wave Equations in Open Channels with Varying Width

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Finite volume methods have proven themselves a powerful tool for finding solutions to the shallow water wave equations. They tend to do well at capturing shocks and are conservative in nature. However one aspect that causes problems is the resolution of steady or near steady states where there is non constant bathymetry. Methods that exactly reproduce the steady state have been called well-balanced. In this work we are interested in a well-balanced scheme for the one dimensional shallow water wave equations but with a modification that allows varying width. Here the well balanced method developed in Audusse is is extended to the equations with varying width. Numerical validation of this method is then provided.

Monday 11:20–11:40 Webster B

A Numerical Study on an Influenza Epidemic Model with Vaccination and Diffusion

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A vaccinated diffusive compartmental epidemic model is developed to explore the impact of vaccination as well as diffusion on the transmission dynamics of influenza. The basic reproduction numbers with and without vaccination are obtained. Stability analysis of the points of equilibrium has been investigated. Using the combined effect of the vaccine efficacy and vaccination rate, the model is analysed to determine criteria for control of influenza epidemic. The roles of vaccine efficacy and vaccination rate are compared. It is shown that higher levels of vaccine efficacy and vaccination rate lead to a decrease in the epidemic size. It is shown that an accurate estimation of the efficiency of vaccine is necessary to control the spread of influenza and thus vaccination strategy needs to be implemented carefully.

Tuesday 12:00–12:20 Webster 251

Analysing Instability of Combustion Waves via Evans Function

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We consider travelling wave solutions of a reaction-diffusion system corresponding to a single-step homogeneous premixed combustion scheme with Newtonian heat-loss and general Lewis number. Properties of the travelling combustion fronts, such as the wave speed, the maximum temperature, the residual amount of fuel that remains behind the reaction front and extinction conditions are derived numerically over a range of different parameter values. Particular attention is paid to unstable combustion wave regimes, especially those associated with oscillatory behaviour. The instability analysis is conducted with the use of Evans function techniques, which we use to derive eigenvalues of the linear stability problem via the use of the argument principle and Nyquist plots. These techniques permit the study of transitions to different modes of unstable behaviour in great detail. Threshold values of the parameters corresponding to Hopf and Bogdanov-Takens bifurcation are established and it is shown that for Lewis numbers above the Bogdanov-Takens threshold value the systems exhibit a period-doubling route to chaotic behaviour.

Tuesday 2:40–3:00 Webster 251

Perturbation Analysis of the Flow of A Powell-Eyring Fluid Between Coaxial Cylinders

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The Powell-Eyring generalized viscous fluid model was developed to model the flow of viscous inelastic shear thinning fluids, such as polymer melts and suspensions of solids in non-Newtonian solvents, giving results showing good agreement with data in the literature for a wide range of fluids. In this paper, we consider the helical flow of a Powell-Eyring fluid between infinitely long coaxial cylinders, with an axial fluid velocity superimposed on a transverse rotational flow. Such a flow, is of relevance to a number of applications, including rheometry. When the intercylindrical gap is small and fluid shear rates are large, we show that a perturbation approach to the flow problem yields simple explicit expressions for the fluid velocity field . These may then be applied to obtain analogous expressions for the viscosity profile in the intercylindrical gap, local stress components and other velocity field functionals.

Monday 11:20–11:40 Webster 250

Use of a Preconditioner for Deflated GMRES(m, k) Method

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GMRES methods are significantly used for Krylov subspace solution of large sparse linear systems of the form Ax=b. The standard procedure consists in restarting the method, when a maximum subspace dimension is reached. More precisely, after say m iterations. However, the restarted version is denoted GMRES(m) slows down its convergence. Recently, a number of techniques that improve the convergence of GMRES(m) method have been proposed. Morgan proposed a procedure, called Deflated GMRES(m, k) method [SIAM J. Sci. Comput. 24 (2002), pp. 20-37]. This method is deflating the k smallest eigenvalues and improving the eigenvalue distribution. The deflating procedure performs by putting harmonic Ritz vectors into the subspace, and this subspace maintains Krylov subspace. In this case, a preconditioning is applied to original linear systems of equations and we consider that we use Deflated GMRES(m, k) method to solve better linear systems of equations. Although several preconditioning techniques can be found in many numerical research papers, we use the proposed preconditioning by J. Erhel [J. Comput. Appl. Math. 69 (1996), pp. 303-318]. This technique is that the smallest eigenvalues of original linear systems replace the largest modulus of the eigenvalues. A preconditioning matrix is effectively computed using GMRES cycle. Moreover, we can also compute using harmonic Ritz vectors. We call this procedure, Deflated GMRES(m, k, l) method. At last, we will present numerical experiments.

Tuesday 12:00–12:20 Webster 250

Modelling Banding Effect and Tag Loss for Little Penguins Using Matlab

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This paper presents a framework for using Matlab to analyse mark-recapture-recovery data arising from studies that use more than one type of tag or multiple tags to mark animals for later identification. It considers life history data collected for groups of single- and double-tagged birds, and forms the likelihood by taking the product of the likelihood contributions for each group. While many studies assume that tags are permanently retained by the birds, such an assumption can result in biased survival estimates. Here life history data from the double-tagged group are used to estimate the tag retention probabilities, and these are incorporated into the likelihood. We illustrate our methods by analysing seven years of mark-recapture data for 2483 Little Penguins Eudyptula minor marked as adults on Phillip Island, Victoria. The intention of this study was to test the effects of banding on the survival of adult penguins which is relevant to the future use of banding as a method for studying Little Penguin biology. We consider data for three groups of birds: one flipper-banded group, one unbanded group that had been implanted with transponders, and one flipper-banded group that had also been fitted with transponders.

Tuesday 4:40–5:00 Webster 251

Biomechanical Behavior of a Femur Following Internal Fixation

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This study carries out a finite element analysis to establish the effect of load conditions and implant material properties on biomechanical behavior of the femur after internal fixation. Two important load configurations are chosen; replicating, stance phase of normal gait cycle as well as, a fall to the side with the force on greater trochanter. A three-dimensional model of dynamic hip screw is created and implanted within a three-dimensional finite element model of intact femur. Two different materials are assigned to dynamic hip screw finite element model for analysis, including stainless steel and titanium alloy. Stress and deflection of the femur and implant is investigated during fall and gait. The results show that under loading conditions, the implanted femur experiences more stresses compared to the intact femur. However large stresses are concentrated within the implant itself. Titanium alloy implant decreases the stress levels within the implanted femur by an average of 40% comparing to the stainless steel implant.

Monday 4:40–5:00 Webster 250

A Multigrid Approach to Visual Cortex Mapping

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A commonly utilised approach in visual cortex mapping calculations involves the unconstrained minimisation of an objective function, representing competing cortical demands of continuity and diversity. The quantities of interest in such calculations, namely neuronal preferences for orientation, position and other visual attributes, reside on a regular mesh, offering natural candidates for multigrid operations. Previous fine mesh calculations employing conjugate gradient iteration, characterised by long and arduous trajectories, have effectively been rendered obsolete by the application of a multigrid approach, which has penetrated deeper into the objective function at a fraction of the computational cost. This paper will describe how the implementation of conjugate gradient and related schemes in a multigrid mode can achieve substantial computational savings in visual cortex mapping calculations, with little modification required.

Monday 2:40–3:00 Webster 251

Ensemble Calculations for Medium Range Weather Prediction

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Numerical weather forecasts are generated by imperfect dynamical models starting from uncertain initial conditions, producing familiar consequences. Ensemble forecasts attempt to capture and quantify the inevitable error behaviour, via a strictly limited family of forecasts, originating from carefully constructed perturbations to the underlying model and/or initial conditions. In the regional context, involving high spatial resolution on a limited domain, additional complexity arises in the treatment of lateral boundary conditions, due to disparity with the coarser global host grid. This paper will describe and demonstrate the operation of a 24 member ensemble under development for medium range forecasting over the Australian region. Typical ensemble performance measures will be discussed, and future scope for enhancement will also be considered.

Monday 10:20–10:40 Webster B

A Large-Scale Genome Simulation Model for the Australian Dairy Cattle Population

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The genome wide association studies generate a large number of hypothesis tests simultaneously, with each hypothesis being the existence or otherwise of an association between the trait and the SNP. The False Discovery Rate (FDR) controlling procedures can be used to tackle this multiple testing problem. The correlation between the tests will affect the estimation of FDR. The Linkage disequilibrium (LD) can influence the correlation between the tests, so the interest here is to investigate how LD affects the reliable identification of true SNP-trait associations based on the Australian dairy cattle population, and this is undertaken by means of a simulation study. The aim of this simulation study is to make a simulated population match to the LD structure of the Australian dairy cattle population. The model adopted forward simulation of population and included the parameters for mutation, varied recombination rate along the chromosome, migration and base gamete population size etc.. The best simulation scenario with the closest LD pattern was found by combining the different parameter settings. FORTRAN language is applied for the computational demanding of this simulation study. Although this model was developed for the Australian dairy cattle population, it is still applicable for human population. What is needed to be done is to alter the simulation parameters to get the similar LD pattern as that of human population.

Monday 11:40–12:00 Webster 251

Stability Analysis of Symplectic Integrators

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In this talk, I will introduce some recent results about the stability of symplectic integrators. The nonlinear stability of symplectic integrators induced by simulating a kind of Hamiltonian systems with a homoclinic orbit. The nonlinear stability is tested by a nonlinear Hamiltonian system of one degree of freedom with one homoclinic orbit. The nonlinear stability set is given by calculating the critical value of step size which generates a homoclinic orbit through the preserved hyperbolic equilibrium of the truncated modified equation of the considered symplectic algorithm. We also present primary relations between the linear stability and the nonlinear stability of symplectic algorithms.

Monday 3:00–3:20 Webster 250

A Projection Method for the Solution of Discrete Thin Plate Splines

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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. Traditional thin plate splines use radial basis functions that produce dense linear system of equations whose size increases with the number of data points. This limits the use of such techniques. We present a discrete thin-plate spline method that uses piecewise functions with local support defined on a finite element mesh. The advantage of using functions with local support is that the dimension of the resulting system of sparse equations depends only on the number of grid points in the finite element mesh, not the number of data points. Another advantage is that an iterative solver, such as the conjugate gradient method, can be used to solve the system. This is an extension on work presented at previous CTAC conferences.

Monday 2:40–3:00 Webster 250

Wavelet Method for Solving the Chemical Master Equation

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It is well known that many realistic mathematical models of biological and chemical systems, such as enzyme cascades and gene regulatory networks, need to include stochasticity. These systems can be described as Markov processes and are modeled using the Chemical Master Equation (CME). The CME is a differential-difference equation (continuous in time and discrete in the state space) for the probability of certain state at a given time. The state space is the population count of species in the system. A upcoming method in solving the CME is to solve for its wavelet approximation. We find that mapping the CME into a wavelet framework reduces the dimension of the problem to compute. However there is an extra computational overhead in finding the right subspace for the solution of wavelet approximation to exist in. The literature points to using the wavelet transform to compute to help deduce which basis functions are needed. However in this method we will propose a new way of finding the subspace we can find the solution of the CME.

Tuesday 10:40–11:00 Webster 251

Reconstruction of Signals with Non-Sparse Components via Compressed Sensing

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We consider the restoration of signals and images which are a combination of a non-sparse function plus a sparse component. These kinds of signals cannot be directly reconstructed using compressed sensing. A new algorithm is presented which aims to reconstruct signals of this type from a limited set of observed data. The algorithm is broken down into two sub-problems which both involve minimization of an l1-regularized least squares problem. Numerical results are presented which demonstrate the effectiveness of the proposed method.

Tuesday 10:20–10:40 Webster 250

CVaR-Minimising Hedging via Smooth Approximation as an Alternative to Discrete Delta-Gamma Hedging

Tanya Tarnopolskaya, Zili Zhu
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This paper studies risk-minimising hedging, and uses conditional value-at-risk (CVaR) as a risk measure. This approach is an alternative to the conventional discrete Delta-Gamma hedging. CVaR minimisation is a non-smooth stochastic minimisation problem, and the non-smoothness is caused by a max-function. The method based on a smoothing approximation for a max-function is potentially more efficient than a standard linear programming approach when the number of Monte-Carlo simulations is large. This paper investigates the performance of the algorithms based on several different smoothing approximations, and compares them with the performance of the algorithm based on linear programming approach. The performance of one period delta-gamma and the CVaR-minimising hedges are compared in this paper. The main advantage of using CVaR-minimising hedge over the Delta-Gamma hedge is the reduction in both the magnitude and the probability of large losses in a portfolio. However, this reduction is often achieved at the expense of a deteriorated expected profit and increased variance of the portfolio loss-distribution. In this paper, we identify situations when CVaR-minimising hedge outperforms delta-gamma hedge according to all performance criteria. The results of this paper suggest that CVaR-minimising hedge based on smooth approximation may provide an efficient and robust alternative to conventional delta-gamma hedge in a high volatility environment.

Tuesday 3:20–3:40 Webster 250

Singular Arcs in Optimal Collision Avoidance Strategies for a Planar Close Proximity Encounter

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Close proximity encounters (i.e., when the participants are sufficiently close in space and time to be of operational concern) occur in many situations in aviation, navigation and robotics. It is known that in the case of participants with equal linear speeds, only nonsingular collision avoidance strategies are optimal. However, as has been shown recently, nonsingular collision avoidance strategies may not be optimal when the participants have unequal linear speeds. This paper explores the possibility of singular arcs for collision avoidance of the participants with unequal linear speeds in a planar close proximity encounter. This problem is a continuous optimal control problem characterised by a free terminal time, a three-dimensional state vector and a terminal cost objective function. The performance objective is to maximize the distance between the participants at the terminal time. We prove that, when one of the participants follows the nonsingular control strategy, the only possible optimal singular strategy for the other participant is a zero control strategy. The results of numerical simulations suggest that zero control strategy for the faster participant cannot be optimal. However, a zero control strategy for the slower participant, with an appropriate choice of the switching time, can improve the performance criterion compared to a nonsingular strategy. Numerical simulations show that the performance criterion as a function of switching time exhibits a maximum.

Monday 3:20–3:40 Webster 251

Comparison of Range Arithmetic Methods in Symbolic-Numeric Circuit Analysis Applications

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In this paper we compare the performance of several range arithmetic methods in evaluating problems in symbolic-numeric circuit analysis. Symbolic-numeric circuit analysis involves solving systems of linear equations in order to obtain the values of currents and voltages in a given circuit. Symbolic circuit expressions contain a large number of product terms and long chains of arithmetic operations which make computations difficult. When analysis of circuit behaviour over a range of parameter values is required the symbolic expressions can be evaluated using one of the range arithmetic methods reported in literature. The range arithmetic methods considered in this paper are affine arithmetic (AA), Extensions to AA (EAA) suggested by Messine, and generalized interval arithmetic (GIA) suggested by Kolev. One important difference between these range arithmetic methods is the way two affine numbers or two generalized interval numbers are multiplied. In this paper, each range arithmetic method is evaluated based on the performance of multiplication operation which is predominant in symbolic circuit expressions. We show that the performance of multiplication rule in each method determines the accuracy of computations. We present the benefits and problems associated with using each of the range arithmetic methods. We also show that GIA gives tighter bounds and efficiently simulates the effects of uncertainties in circuit parameters when solving problems in circuit analysis.

Monday 5:00–5:20 Webster 251

Study on Biodegradation of Xenobiotic Polymers with Change of Microbial Population

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Microbial depolymerization processes are classified into two types, the exogenous type and the endogenous type. In an exogenous type depolymerization process, monomer units are separated from terminals of molecules stepwise. Examples of polymers subject to exogenous type depolymerization processes include polyethylene and polyethylene glycol. In an endogenous type depolymerization process, molecules are cleaved at any positions. Examples of polymers subject to endogenous type depolymerization processes include polyvinyl alcohol and poly lactic acid. In this study, growth of microbial population is taken into account to simulate biodegradation process of xenobiotic polymers. A mathematical model for depolymerization process is described. It consists of differential equations for which the weight distribution with respect to molecular weight and the microbial population are unknown function of time. The degradation rate is a product of a molecular factor and a time factor. An inverse problem is solved to determine the molecular factor. The time factor is the microbial population which grows under sufficient supply of carbon source, and which diminishes as the carbon source is exhausted.

Wednesday 10:00–10:20 Webster 251

Stability Characteristics of Conjugate Natural Convection Boundary Layers

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In this study the stability characteristics of conjugate natural convection boundary layers are examined numerically by simulating the flow formed in two adjacent two-dimensional rectangular cavities joined along one vertical wall. The outer vertical walls are isothermal, with one 'hot' wall and one 'cold' wall. The vertical wall that separates the two joined cavities has an infinite conductivity and the horizontal walls are adiabatic. Heat is transfered between the cavities through the conducting wall so boundary layers are formed on all the vertical walls. The boundary layers on either side of the conducting plate flow in opposite directions and interact through the temperature field. This interaction is a feedback mechanism which allows the system to become absolutely unstable above a critical Rayleigh number. Simulations in this study indicate that this critical value is Ra $= 1.2 * 10^{10}$ at Prandtl number of Pr=7.5 , where H is the height of the cavity. The characteristics of the flow are examined by first obtaining the steady mean base-flow for the cavity by numerically solving the full Navier-Stokes equations. We then simulate numerically only a perturbation applied to this base-flow. The results illustrate how the perturbations are amplified along the boundary layer and perturb the opposing boundary layer.

Tuesday 11:40–12:00 Webster B

Free-Surface Flow Under a Sluice Gate of an Inclined Wall from Deep Water

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Nonlinear solutions of free surface flow under a sluice gate are studied in this paper. Upstream, the fluid is assumed to be infinitely in depth, and the gate makes an angle β to the horizontal axis. Therefore, the flow emerges from the gate and produces uniform stream far downstream. The problem is solved numerically by a boundary element method derived from an integral equation along the free surface. An analytical function is constructed, relating to the upstream flow, so that the integral equation is solvable. As the result, a free surface flow with smooth detachment from the edge of the gate is obtained for relatively large upstream Froude numbers, otherwise a free surface with back flow near the edge of the gate is indicated, and it tends to a stagnation point for a certain Froude number.

Tuesday 10:40–11:00 Webster B

Transition from Laminar to Unstable Flow by a Fin on the Sidewall of a Differentially Heated Cavity

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We investigate the transition from a laminar to an unstable flow induced by a fin on the sidewall of a differentially heated cavity (a prototype of many industrial heat exchangers), using direct numerical simulation. In this paper, a wide range of Rayleigh numbers and different fin lengths with Pr = 6.63 are considered. It is found that the flow adjacent to the finned sidewall is stable for the cases with global Rayleigh numbers lower than a critical value and unstable for those with global Rayleigh numbers higher than a critical value. Such an unstable flow results from a fluid layer above the fin with an adverse temperature gradient, which is verified to be a Rayleigh-Benard-Poiseuille flow, and the transition from a steady laminar to an unstable flow is determined by the local Reynolds number and local Rayleigh number and in turn the fin length and global Rayleigh number. Furthermore, features of the unstable flow induced by the fin are characterized.

Tuesday 12:20–12:40 Webster B

Novel Numerical Methods for Nonlinear Time-Space Fractional Diffusion Equations in Two Dimensions

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In this paper, nonlinear time-space fractional diffusion equations in two dimensions (NTSFDE-2D) are considered. The NTSFDE-2D is obtained from the standard diffusion equation by replacing the first-order time derivative with the Caputo fractional derivative, and the second order space derivatives with the fractional Laplacian. Using the matrix transfer technique (MTT) proposed by Ilic, Liu, Turner, and Anh (2006, Fractional Calculus and Applied Analysis, 9, 333-349), the NTSFDE-2D is transformed into a time fractional differential system, where A is the approximate matrix representation of the standard Laplacian. Traditional approximation of the fractional Laplacian requires diagonalisation of A, which is very time-consuming for large matrices. The novelty of our proposed numerical scheme is that, using the finite difference method to approximate the Caputo time fractional derivative, the solution of the NTSFDE-2D is written in terms of a matrix function vector product at each time step. We use the finite volume method over unstructured meshes to generate the matrix A, and the Lanczos method to approximate the matrix function vector product. Numerical results are presented to verify the accuracy and efficiency of the proposed numerical solution strategies.

Tuesday 4:00–4:20 Webster 250

Computational Simulation of Connectivity in the Brain Using Full Diffusion Tensor from MRI

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Diffusion tensor magnetic resonance image (DT-MRI) is a technique used to measure the diffusion properties of water molecules in tissues. Anisotropic diffusion can be described by the equation

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C)$$

where C is the concentration of water molecules and D is a diffusion tensor. The anisotropy of the diffusion tensor is of particular interest in brain images, as it is related to fibre tracts in white matter. Depending on the interrelation of the eigenvalues of D, diffusion can be divided into linear, planar and spherical diffusion. In this paper we present the maps of diffusion tensor, fractional anisotropy, relative anisotropy, volume ratio, tensor trace and colour-coded orientation calculated from the image of brain of a patient with Parkinson's disease that can be derived from the diffusion tensor. We propose computational simulations of connectivity in the brain using finite element methods for the analysis of DT-MRI. This method involves solving a diffusion equation based on the measured diffusion tensor, where the initial condition is a seed at a point that would be located as a starting point in tractography. The seed diffuses through the brain, and the amount of diffusion at some position is interpreted as a probability to reach that point, given the input data. Our method calculates connection probabilities between points of interest, which can be compared within, or between, brain images.

Tuesday 4:00–4:20 Webster 251

The Lattice Boltzmann Method for Laminar and Turbulent Channel Flows

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Plane Poiseuille channel flows are simulated using the Lattice Bhatnagar Gross Krook (LBGK) method, the simplest Lattice Boltzmann Method (LBM). The flow is driven by a body force in a periodic domain. Low Reynolds number flows are tested for asymptotic convergence in 2D and the results verified in 3D. Turbulent flows are benchmarked against published direct numerical simulation results. A regularization scheme is evaluated as a means of stabilizing the scheme at Reynolds numbers higher than 20,000. We aim to determine whether the LBGK method is an effective tool to continue research into fundamental turbulent flows. The success of the LBM is judged based on accuracy, stability, numerical efficiency and parallel efficiency. Compressibility error caused problems in the search for asymptotic convergence and, as expected, we encountered instabilities at higher Reynolds numbers. Entropy and other "ghost" properties of the particle distribution are encountered are used to motivate stabilization methods. The LBGK method has limited application as a raw method. Our aim is to develop a highly scalable fluid dynamics code through a balance between additional complexity and the above concerns. We present a range of applications for the LBGK method and give details of where it falls short. This work will be used as a guide to what Reynolds numbers are achievable using the standard LBGK method and also as a supplement to other papers dealing with stabilization methods.

Tuesday 10:20–10:40 Webster B

Inverse Method for Attribution of Climate Change

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A new inverse method is developed for attributing the anomalous forcing functions responsible for the changes in the statistical means, or climate states, of atmospheric observations and simulations. Attributing the causes of observed climate change to a variety of physical and dynamical processes is a contemporary problem of great significance in climate science. Mathematically the inversion problem to find the anomalous forcing functions is a difficult one because it relies on a solution to the turbulence closure problem. The equation for the statistical mean climate state involves the covariance of fluctuations and the covariance or two-point function in turn involves the three-point function and so on to all orders. Here we employ a method motivated by recent advances in closure theory for inhomogeneous turbulence that expresses the covariance of fluctuations as a linear term in the statistical mean state and a constant term. We apply the method to climates obtained from the statistics of direct numerical simulations of atmospheric circulations during the second half of the 20th century. The anomalous forcing functions responsible for dramatic changes in the southern hemisphere climate since the mid-1970s are calculated using this method. We demonstrate that the forcing functions, from which climate change may be attributed, are in very good agreement with the forcing functions used in simulations of observed climate states during the 20th century.

Monday 2:40–3:00 Webster B

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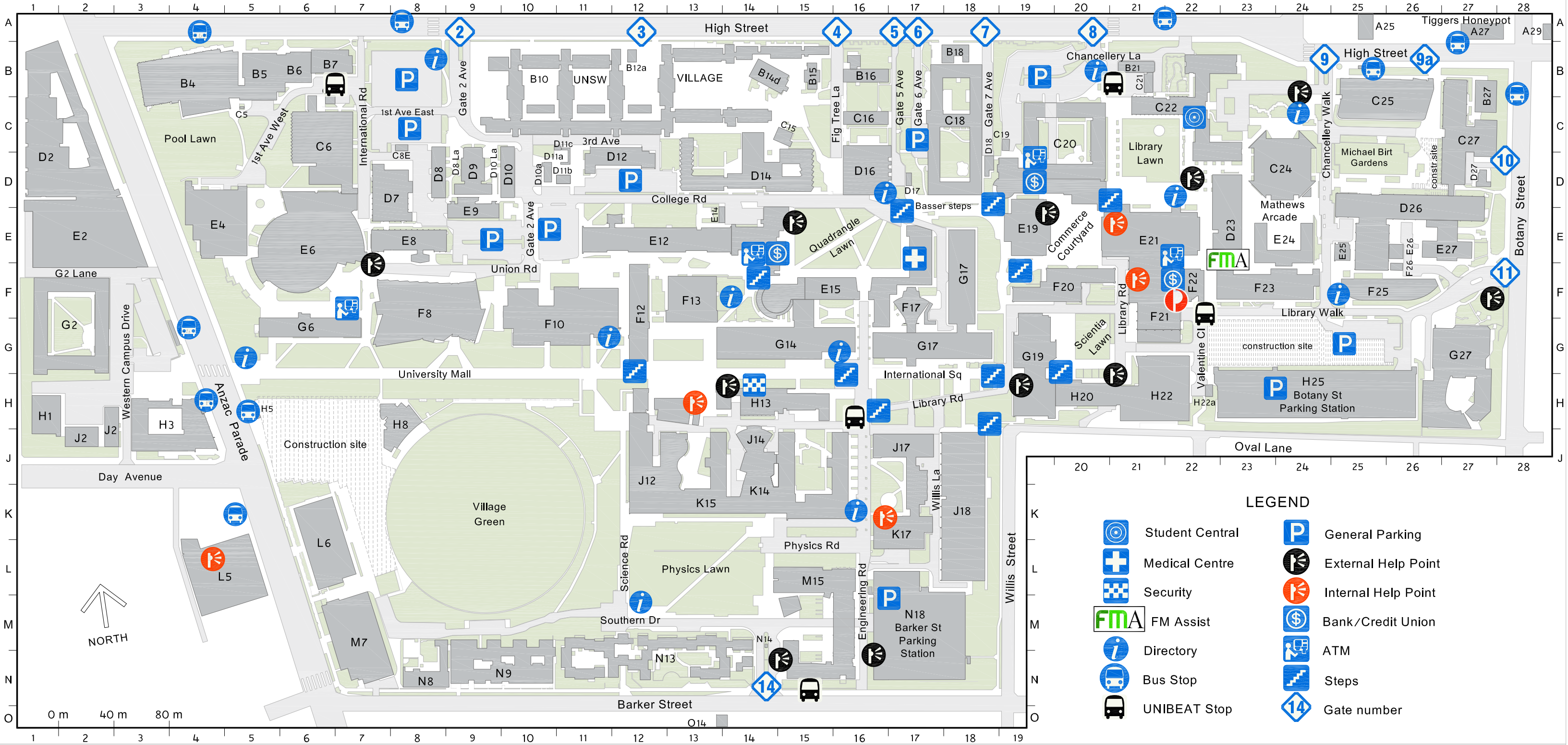

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