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CTAC'08 Conference Abstracts  
Bishnu Lamichhane, Paul Leopardi & Linda Stals (Editors)



# Contents

<b>1 Committees</b>	<b>2</b>
<b>2 Abstracts of invited presentations</b>	<b>3</b>
<b>3 Abstracts of contributed presentations</b>	<b>9</b>
<b>Index</b>	<b>52</b>



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# Abstracts of invited presentations



# Nonconforming Methods for Electromagnetics

Susanne Brenner  
Louisiana State University, USA  
Email: brenner@math.lsu.edu

In this talk we will discuss several new nonconforming finite element methods for electromagnetic problems formulated in subspaces of the intersection of  $H(\text{curl})$  and  $H(\text{div})$ , where the problems become elliptic. Both theoretical and numerical results will be presented.

# Spectral Methods for Time-Dependent Free-Surface Problems in Fluid Mechanics

Larry Forbes  
University of Tasmania, Australia  
Email: Larry.Forbes@utas.edu.au

Free-surface flows in fluid mechanics are among the most difficult problems to solve mathematically, and they have engaged researchers for at least the last 150 years. Their difficulty comes from the fact that they are inherently non-linear, since the shape of the region occupied by the fluid is itself part of the problem to be solved.

In past two decades, some steady-state (time independent) free-surface problems in fluid mechanics have been able to be solved numerically. Typically, the fluid is assumed to be ideal (not viscous), so that Laplace's equation for a velocity potential holds throughout the fluid. The problem is nevertheless still highly non-linear, since the free-surface location remains unknown initially. In recent years, however, it has become apparent that steady-state solutions leave many questions unanswered. In particular, it is sometimes not clear if those solutions would be stable to small disturbances, or if they could even be reached at all in a time-dependent problem that starts from sensible initial conditions.

In this talk, we will present a new spectral method for solving some free-surface flows in ideal fluids. The method makes use of a basic Fourier-series type representation of the solution with time-dependent coefficients. It is then possible to derive elegant identities involving the Fourier coefficients along the free surface, and these lead to a highly efficient set of ordinary differential equations for the coefficients, that can be solved to high accuracy. We will illustrate the method by reference to some practical problems in the draining of a tank of water, and resonant sloshing in a tank forced horizontally. We will also consider the famous Rayleigh-Taylor instability, in which a heavy fluid lies above a light fluid. Spectral methods have been developed for this problem in both the ideal and the viscous fluid cases, and reveal some interesting behaviour as the instability develops and grows.

# Petaflops, Seriously

David Keyes  
Columbia University, USA  
Email: david.keyes@columbia.edu

Sustained floating-point rates on real applications, as tracked by the Gordon Bell Prize, have increased by over five orders of magnitude from 1988, when 1 Gigaflop/s was reported on a structural simulation, to the 200 Teraflop/s recently reported on a molecular dynamics simulation. Various versions of Moore's Law over the same interval provide only two to three orders of magnitude of improvement for an individual processor; the remaining factor comes from concurrency, which is of order 100,000 for the BlueGene/L computer, the platform of choice for the majority of recent Bell Prize finalists. As the semiconductor industry begins to slip relative to its own roadmap for silicon-based logic and memory, concurrency has played an increasing role in attaining the next order of magnitude, the long-awaited milestone of 1 Petaflop/s (one million Gigaflop/s), which occurred in June 2008 for the ScaLAPACK benchmark on Roadrunner at Los Alamos National Laboratory, and should be demonstrated on a practical application during 2009.

Simulations based partial differential equations (PDEs), such as fluid dynamics or electromagnetics, can be among the first applications to take advantage of petascale capabilities, but not the way most are presently being pursued. Only "weak scaling" can get around the fundamental limitation expressed in Amdahl's Law (1967) and only optimal implicit formulations can get around another limitation on scaling that is an immediate consequence of Courant-Friedrichs-Lewy stability theory (1928) under weak scaling of a PDE. Many PDE-based applications and other lattice-based applications with petascale roadmaps, such as quantum chromodynamics, will likely be forced to adopt optimal implicit solvers. However, even this narrow path to petascale simulation is made treacherous by the imperative of dynamic adaptivity, which drives us to consider algorithms and queueing policies that are less synchronous than those in common use today. Drawing on the ScaLeS report (2003-04), the latest ITRS roadmap, some back-of-the-envelope estimates, and numerical experiences with PDE-based codes on recently available platforms, we will attempt to project the pathway to Petaflop/s for representative applications.

# Computational Methods for Phase Response Analysis of Circadian Clocks

Linda Petzold  
University of California, USA  
Email: petzold@engineering.ucsb.edu

Circadian clocks govern daily behaviors of organisms in all kingdoms of life. In mammals, the master clock resides in the suprachiasmatic nucleus (SCN) of the hypothalamus. It is composed of thousands of neurons, each of which contains a sloppy oscillator - a molecular clock governed by a transcriptional feedback network. Via intercellular signaling, the cell population synchronizes spontaneously, forming a coherent oscillation. This multi-oscillator is then entrained to its environment by the daily light/dark cycle. Both at the cellular and tissular levels, the most important feature of the clock is its ability not simply to keep time, but to adjust its time, or phase, to signals. We present the parametric impulse phase response curve (pIPRC), an analytical analog to the phase response curve (PRC) used experimentally. We use the pIPRC to understand both the consequences of intercellular signaling and the light entrainment process. Further, we determine which model components determine the phase response behavior of a single oscillator by using a novel model reduction technique. We reduce the number of model components while preserving the pIPRC and then incorporate the resultant model into a couple SCN tissue model. Emergent properties, including the ability of the population to synchronize spontaneously are preserved in the reduction. Finally, we present some mathematical tools for the study of synchronization in a network of coupled, noisy oscillators.

# Simulation of Complex Flows with the Lattice Boltzmann Method on Supercomputers

Ulrich Ruede  
University of Erlangen-Nuremberg, Germany  
Email: Ulrich.Ruede@informatik.uni-erlangen.de

The Lattice Boltzmann Method (LBM) is based on a discretization of the Boltzmann equation and results in a cellular automaton that is relatively simple, easy to extend, and well suited for parallelization. In the past few years, the LBM method has been established as an alternative method in computational fluid dynamics. Here, we will discuss extensions of the LBM to compute flows in complex geometries such as blood vessels or porous media, fluid structure interaction problems with moving obstacles, and free surface flows. We will outline the implementation in the waLBERla software framework and speedup results for current parallel hardware. This includes Heterogeneous multicore CPUs, such as the IBM Cell processor, and the implementation on massively parallel systems with thousands of processor cores.

# High-dimensional Challenges for Computational Mathematics

Ian H. Sloan

University of New South Wales, Australia

Email: [i.sloan@unsw.edu.au](mailto:i.sloan@unsw.edu.au)

Richard Bellmann coined the phrase "the curse of dimensionality" to describe the extraordinarily rapid increase in the difficulty of most problems as the number of variables increases. A typical problem is numerical multiple integration. It is clear that the cost of every integration formula of product type rises exponentially with the number of dimensions. Nevertheless, problems with hundreds or even thousands of variables do arise, and are now being tackled successfully. In this talk I will touch briefly on recent advances in understanding and constructing high dimensional integration rules, but much of the focus will be on applications, in diverse fields such as mathematical finance, linear models in statistics, and flow through porous media. A general theme is that high-dimensional problems present an enduring challenge for numerical analysis.

# Efficient Coupling of Finite Elements and Boundary Elements/Adaptive Procedures and Preconditioners

Ernst Stephan  
Institute for Applied Mathematics  
University of Hannover, Germany  
Email: stephan@ifam.uni-hannover.de

We present h- and p-adaptive procedures for the symmetric coupling of finite element and boundary element methods for linear and nonlinear interface problems [1,2]. (Here,  $h$  denotes the mesh size and  $p$  the polynomial degree of the Galerkin solution). Our coupling approach reduces the interface problems to differential equations in a bounded domain  $\Omega$  together with (weakly singular, singular, and hyper singular) boundary integral operators on the boundary of  $\Omega$ . We give two types of a posteriori error estimates a) using hierarchical basis techniques with easily computable local error indicators and b) residual based estimates. The corresponding error controlled adaptive procedures give good meshes and polynomial degree distributions for the h-p version of the coupling, allowing independent refinements of finite elements and boundary elements, leading to efficient numerical procedures. Furthermore, we propose efficient preconditioners for the minimum residual method to solve the indefinite, symmetric systems of equations resulting from the FE/BE coupling yielding (almost) bounded numbers of iterations. Here we use Multigrid, BPX, and Schwarz methods both for finite and boundary elements [3]. We demonstrate the power and the applicability of the FE/BE coupling with the 3D eddy current problem in electromagnetics [4] and the contact problem with friction for two elastic bodies [5,6]. In all cases numerical results are presented which support the theory.

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[2] P. Mund, E.P. Stephan: An adaptive two-level method for the coupling of nonlinear FEM-BEM equations, SIAM J. Numer. Anal. 36 (1999) 1001-1021

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[4] E.P. Stephan, M. Maischak, F. Leydecker: An hp-adaptive finite element/boundary element coupling method for electromagnetic problems, Comput. Mech. 39 (2007)673-680

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# Abstracts of contributed presentations



# A Fully Discrete Algorithm for High Frequency Acoustic Scattering in Three Dimensions

Stuart Hawkins  
School of Mathematics and Statistics  
UNSW, Australia  
Email: stuart.hawkins@unsw.edu.au

Surface integral equation methods are advantageous for simulating scattering of acoustic waves by three dimensional bodies because they efficiently reduce the dimension of the problem. However, in general, the cost of assembling the associated dense scattering matrix grows with increasing frequency because the number of unknowns required to represent the standard physical density depends on the acoustic size  $ka$  of the scatterer, where  $k$  is the wavenumber of the incident radiation and  $a$  is the diameter of the obstacle. In addition, for fully discrete high frequency algorithms, evaluation of a large number (depending on the unknowns) of highly oscillatory singular surface integrals using standard quadrature rules is prohibitive. In this work, we present a novel fully discrete algorithm for three dimensional high frequency acoustic scattering with complexity almost independent (in logarithmic sense) of the acoustic size of convex sound-soft scatterers. We demonstrate the algorithm by simulating sound waves scattered by convex three dimensional bodies with acoustic sizes one hundred to one million, with CPU time almost independent of the acoustic sizes. This is a joint work with M. Ganesh.

# A Method for Estimating the Potential Predictability of Precipitation over Western Australia

Carsten Frederiksen  
Bureau of Meteorology, Australia  
Email: c.frederiksen@bom.gov.au

A number of recent studies have provided a method for estimating the potential predictability of seasonal mean climate variables using monthly data. The methodology separates the inter-annual variance of the climate variable into an unpredictable and predictable component. For seasonal mean variability, these are known as the intraseasonal and slow component, respectively. The ratio of the total to the slow variance is a measure of the potential predictability. The methodology assumes that the monthly statistics of the climate variable are stationary and the underlying daily time series is a first order autoregressive process. These assumptions do not hold for a variable such as precipitation where the daily data consists of dichotomous (yes/no) events. Here, we propose a method that allows for such two state climate variables. The method relies on determining an estimate for the inter-month autocorrelations for precipitation. We use a stochastic two-state first-order Markov chain model fitted to the daily data. Estimates of the transition probabilities, and the long-run relative frequencies of the two states, for each month, are made from multi-decadal time series of daily precipitation data. Once the inter-month autocorrelation has been estimated, the intraseasonal and slow components, and hence the potential predictability, can be estimated. Here, we illustrate the methodology by applying it to observed Western Australian precipitation for the period 1951-2000.

# **A Method for Estimating the Potential Predictability of Precipitation over Western Australia**

Simon Grainger  
Bureau of Meteorology, Australia  
Email: S.Grainger@bom.gov.au

The seasonal mean of an atmospheric climate variable can be considered to be a statistical random variable with two components: a ‘slow’ component related to slowly varying (time scales of a season or more) forcings from external and internal atmospheric sources, and an ‘intraseasonal’ component related to forcings from weather variability with time scales less than a season. In this paper, an extension of a method to estimate the ‘intraseasonal’ covariance from monthly moments is described. By removing the ‘intraseasonal’ covariance from the seasonal mean total covariance, an estimate of the residual, ‘slow’ covariance is obtained. Eigenvalue decomposition is applied to the ‘slow’ and ‘intraseasonal’ covariance matrices to obtain the dominant modes of variability (eigenvectors) for observed and modelled atmospheric variables. The relative variance (eigenvalues) and spatial correlation between the dominant modes of variability in models and observations are calculated. The relationship between variance and correlation for each mode of variability can be shown graphically. The results from this method are investigated using monthly 500hPa geopotential height from observations (reanalysis data) and coupled global climate models for the second half of the 20th Century.

# **A Numerical Approach to Modelling Avascular Tumour Evolution with White Noise**

Keng Cheng Ang  
Nanyang Tech. University, Singapore  
Email: kengcheng.ang@nie.edu.sg

In this paper, a model for avascular tumour growth with white noise is presented. The model is essentially formulated as a set of partial differential equations describing the spatio-temporal evolutions of cell concentrations based on reaction-diffusion dynamics and the law of mass conservation. Perturbations in the form of white noise are introduced to model the effects of random processes on distinct time scales. A numerical approach is used to solve the system and numerical simulations in one and two space dimensions are presented. Numerical results indicate that the proposed model is a reasonable approach that may be used to examine the effects of nutrient supply in tumour growth dynamics.

# **A Numerical Solution for Moving Boundary Shallow Water Flow in Parabolic Bottom Topography.**

Joe Sampson  
Swinburne University of Technology, Australia  
Email: jsampson@swin.edu.au

A numerical solution of the nonlinear shallow water wave equations for unforced linear flow above parabolic bottom topography has been found. This solution involves moving shorelines. The motion decays over time. The numerical model used is adapted from the SLM (Selective Lumped Mass) numerical model. The wetting and drying scheme used is different to that in the SLM model. The SLM model is finite element in space, using fixed triangular elements, finite difference in time and is explicit. The numerical solution has been compared with an analytical solution with good agreement between the two solutions.

# **A Petrov-Galerkin Method for an Integro-Differential Equation with a Memory Term**

Kassem Mustapha  
King Fahd University of Petroleum and Minerals  
Saudi Arabia  
Email: kassem@kfupm.edu.sa

In this work we propose and analyse a finite element method for solving an integro-differential equation with a memory term. For the time discretization of the equation, we use a Petrov-Galerkin method with piecewise linear polynomials combined and for spatial discretization we use standard piecewise finite elements. We prove optimal error bound of the discrete solution in the  $L_\infty(L_2)$  and  $L_\infty(H^1)$  norms. We compare the theoretical error bounds with the results of numerical computations.

# **A Posteriori Error Estimates For $H^1$ -Galerkin Mixed Finite Element Methods for Elliptic Problems**

Rajen Sinha  
Department of Mathematics  
IIT Guwahati, India  
Email: rajen@iitg.ernet.in

We study a posteriori error analysis of  $H^1$ -Galerkin mixed finite element methods for second order elliptic partial differential equations. A reliable and efficient error estimators are constructed under a saturated assumption and using a Helmholtz decomposition of vector fields. The present analysis does not require LBB consistency condition.

# A Restarted and Preconditioned Matrix Transfer Technique for Solving the Fractional Poisson Equation

Daniel Simpson  
QUT, Australia  
Email: dp.simpson@qut.edu.au

When considering the steady-state of systems undergoing anomalous diffusion, it is often necessary to solve the fractional Poisson equation (FPE)

$$\begin{aligned} (-\Delta)^{\alpha/2}\phi(x) &= f(x), & x \in \Omega \subset \mathbb{R}^2, \alpha > 0, \\ \phi(x) &= 0, & x \in \partial\Omega, \end{aligned} \tag{3.1}$$

where  $0 \leq \alpha \leq 2$  and the fractional Laplacian  $(-\Delta)^{\alpha/2}$  is defined using the spectral representation of  $(-\Delta)$  on  $\Omega$ . In this paper we will investigate a novel method, known as the Matrix Transfer Technique (MTT), for approximating the solution to (3.1). Given an underlying discretisation scheme for solving the standard Poisson equation, the MTT is constructed using the discretised Laplacian  $A_n$ , assumed here to be symmetric and positive definite. The approximate solution to (3.1) is defined as  $\phi_n = A^{-\alpha/2}\bar{f}$ , where  $\bar{f}$  is the projection of  $f$  onto the approximation space. In practice,  $A_n$  is a large, sparse, SPD matrix and, therefore,  $\phi_n$  is often computed using a restarted and preconditioned Lanczos approximation. In this talk, we will apply a number of restart and preconditioning schemes from the literature to this problem for general  $\alpha$ . In particular, we will investigate the application of the shift-and-invert preconditioning method to this problem.

## A Spectral Method with Quadrature for Navier-Stokes Equations on the Rotating Sphere

Quoc Thong Le Gia  
School of Mathematics and Statistics  
University of New South Wales, Australia  
Email: qlegia@maths.unsw.edu.au

Numerical algorithms for partial differential equations (PDEs) posed on the surface of spherical geometries play an important role in addressing fundamental error issues in various circulation and gravitational potential research models on the rotating Earth. In particular, the flows in the atmosphere are considered to be accurately modeled by the Navier-Stokes PDEs on the rotating sphere. In this work, we describe, analyze, and implement a quadrature spectral method for a global computer modeling of the incompressible Navier-Stokes PDEs on the rotating unit sphere. This is joint work with M.Ganesh and I.Sloan.

# **A Spring and Mass Model for Determining the Lowest Risk Path in a Threat Environment**

Martin Rowe  
UNSW@ADFA, Australia  
Email: m.rowe@student.adfa.edu.au

A fundamental problem for the military is finding the safest path through a dangerous area. The problem is common to all branches of the military, for example aircraft need to avoid enemy radars to remain undetected and ships and vehicles must avoid going near mines. Finding the safest path through these threats is essential in ensuring that military members are not put in needless danger. The consequences of choosing a bad path in these situations can often be fatal. Currently the main method of finding the safest path around known threats is using a Voronoi diagram and assigning a threat level to each discrete path. This approach does not scale well to many threats nor is it able to adapt to changing threats because it must recalculate the path from the beginning again. The spring and mass model instead uses a chain of masses connected by springs and a phantom repulsive force between the masses and the threats. Using the equations of motion a series of easily solvable ODEs can be found and the solution to these will be the lowest risk path through the threats. This method quickly finds a solution if the initial values are close to the solution, so the model can easily adapt to changing threats by using the old path as the initial guess for the new path. This work will examine the changing threat problem as well as other areas the spring and mass model can be expanded to include.

# **A Three-Dimensional Finite Volume Method for Modelling Saltwater Intrusion into Coastal Aquifers**

Timothy Moroney  
QUT, Australia  
Email: t.moroney@qut.edu.au

A three-dimensional finite volume model is developed for the simulation of saltwater intrusion into coastal aquifer systems. A pair of coupled, nonlinear equations governing fluid flow and salt transport is discretised over unstructured meshes, and solved in parallel using MPI. The code itself is written in a modular fashion, allowing the same core FVM code to handle different physics, specified at compile time. The impact of mesh element types, mesh refinements, timestepping procedures and convection schemes on the accuracy and efficiency of the method are compared. Results are exhibited for a number of well-known test problems.

# Acceleration of Inexact Inverse Iteration for Eigenvalue Problems

Alan Andrew  
Mathematics Department  
La Trobe University, Australia  
Email: a.andrew@latrobe.edu.au

Many methods have been used to improve the efficiency of iterative numerical algorithms. Combining different methods is not always possible, because the performance of acceleration methods usually depends critically on the precise form of the error in successive iterates, and this form often changes when other acceleration methods are used. Inexact implementation methods have proved particularly effective in increasing the efficiency of iterations involving sparse matrices. This paper investigates the extent to which the efficiency of inexact inverse iteration and the inexact Rayleigh quotient algorithm, for the numerical computation of eigenvalues and eigenvectors of sparse matrices, may be further increased by the use of the scalar epsilon algorithm. Some encouraging numerical results are presented and some pointers are given for future research.

# Adaptive Augmented GMRES Method for Solving Ill-Posed Problems

Nao Kuroiwa  
Keio University, Japan  
Email: bambino\_poo@z5.keio.jp

GMRES method, one of the iterative methods, makes better solution of large linear systems of equations with a non-symmetric coefficient matrix. We now present adaptive augmented GMRES method. The GMRES method generates a Krylov subspace for the solution, and the augmented GMRES method allows augmentation of the Krylov subspaces by user-supplied subspace which represents certain known features of the desired solution. The augmented GMRES method performs well with suitable augmentation, while poorly with unsuitable augmentation. It is very important which subspace to augment the Krylov subspace. However, we are not able to choose the suitable subspace to augment when the features of the desired solution are unknown. The adaptive Augmented GMRES method automatically determines the suitable subspace to augment the Krylov subspace. We show that the method maintains performance of the augmented GMRES and lightens the burden on users. At last, extensive numerical experiments are conducted in order to compare robustness and efficiency of various heuristic strategies.

# **AGREPS: ACCESS Global and Regional Ensemble Prediction Scheme**

Terence O'Kane  
CAWCR Bureau of Meteorology, Australia  
Email: t.okane@bom.gov.au

Deterministic numerical weather forecasts fail over reasonable prediction periods due to the inherent nonlinearity in the system and because of errors in the initial conditions. Recent ensemble forecast methodologies regard weather forecasting as a statistical problem of predicting the probability density function of atmospheric states providing not only improved estimates of the mean but also estimates of the forecast error variance and possibly the higher order moments. In this talk we report on progress in the development of the ACCESS Global and Regional Ensemble Prediction Scheme (AGREPS) at the Bureau of Meteorology. Based on the UK Met office ensemble, AGREPS implements an Ensemble Transform Kalman Filter (ETKF) to generate independent initial perturbations as fast growing disturbances with structures and growth rates typical of the analysis errors. This method allows information about the fast growing errors to be incorporated into the initial perturbations for the forecast, which for particularly dynamic flows arise due to large scale instabilities. An ensemble of model states is propagated using the AGFS/ARFS operational numerical weather prediction system allowing the construction of the forecast error covariance at any given time by averaging over the ensemble. Covariance localization and inflation are implemented to minimise the effect of small sample size.

## **Air Flow Through a Wine Cork**

Steven Barry and Pems South  
UNSW@ADFA, Australia  
Email: s.barry@adfa.edu.au

During transport and storage of wine, temperature differences can cause thermal expansion of the air between the wine and the cork. This causes air flow through the cork which can adversely effect the shelf life of the wine. We explore here models of the air transport, and methods of solution, both numerical and analytic, and the likely effect on wine shelf life.

## **Annealing of Steel Coils**

Steven Barry  
Pems South  
UNSW@ADFA, Australia  
Email: s.barry@adfa.edu.au

Thermal annealing of steel coils is a crucial component of making effective sheet steel. The one tonne coils involve hundreds of layers in a one metre radius. Modelling the heat transport within the coil is made difficult by the non-constant air gap between each steel layer. We explore different ways to model the coil, and some of the complexities in numerically calculating solutions.

# **Application of Method of False Transients to Generate Smooth around a Body in Motion Grids**

Eddie Ly  
Rmit University, Australia  
Email: eddie.ly@rmit.edu.au

A procedure for automatic numerical generation of a structured grid system with coordinate lines coincide with all boundaries of a general two-dimensional region containing a body in motion is presented. No restrictions are enforced on the shape of the boundaries, which may even be time dependent, and the approach can be extended to generating grids for body of arbitrary shapes in three dimensions. The solution procedure incorporated the method of false transients and the approximate factorisation algorithm, where a sequence of time steps is cycled in a geometric fashion with repeated endpoints, and has a capability for clustering grid lines close to the body. The procedure requires significantly much less computational effort to obtain a converged solution than a point or line successive over-relaxation iterative scheme. It was observed that if the employed numerical scheme is numerically stable and converged, a correct final grid system can always be obtained independent of the form of its initial grid system, and hence, make it suitable for automatic dynamic grid generation computer code. Although, the superiority of the presented algorithm has been demonstrated for the grid generation problem, it can be utilised for other problems requiring the solution of a set of elliptic partial differential equations of similar nature.

# **Application of Rational Chebyshev and Hermite Polynomials to Optical Problems**

Isaac Towers  
UNSW@ADFA, Australia  
Email: i.towers@adfa.edu.au

Many problems in optics involve propagating a field forward in time/space and simulating how it behaves in a nonlinear medium. Such problems often have, in theory, boundary conditions at infinity. Traditionally, when solving the underlying PDE of the problem, one discretises the transverse dimension(s) with finite differences or Fourier modes and propagates the field using some kind of explicit or implicit scheme. The domain of the problem is truncated to a suitably large size which allows the boundary conditions to be approximated. We assess the use of Hermite and the so-call rational (or stretched) Chebyshev polynomials, both with infinite domain, for discretising the transverse dimension(s) of such propagation problems. The nature of these polynomials allows one to handle the boundary conditions with greater correctness. The field is propagated forward by exponential integration and the results are compared to more commonly used operator splitting techniques.

# **Application of the Variational Iteration Method to the Bonhoeffer Van Der Pol Equation**

Richard Pennifold  
UNSW@ADFA, Australia  
Email: r.pennifold@adfa.edu.au

Nonlinear dynamical systems rarely have a nice closed form solution. It is therefore necessary to approximate the solution analytically or compute a solution numerically. Traditionally perturbation theory has featured in the analytic approach to the solution nonlinear dynamical systems however this requires the systems to have a ‘small’ parameter which can be exploited via a perturbation expansion. Recently there have been a number of analytic approximation techniques developed to address problems exhibiting strong nonlinearities, in particular He’s Variational Iteration Method (VIM). This talk will describe the authors’ work applying these new methods to the Forced Bonhoeffer van der Pol equations and other related equations. Difficulties due to the periodic nature of these equations will be highlighted.

# **Approximating the Solution of the Chemical Master Equation by Aggregation**

Markus Hegland  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: markus.hegland@anu.edu.au

The chemical master equation (CME) is a continuous time discrete space Markov model of chemical reactions. It is used in preference to the (deterministic) kinetic rate equations when the copy numbers of the species involved are low. In this case noise is an important driver of the reactions. Applications include gene regulatory networks and signalling networks in molecular biology. The numerical solution of the CME discussed here is based on state space aggregation and piecewise polynomial disaggregation. We will provide new error bounds for this solution. In particular, we will discuss the issues raised by high dimensionality which occurs for systems involving a large number of species. We will compare the numerical solution of the CME with alternative methods based on simulation, i.e., Monte Carlo. This is joint work with Per Loetstedt, Uppsala.

# Association Rule Mining in Magnetic Confinement Fusion Data

Frank Detering  
Australian National University, Australia  
Email: frank.detering@anu.edu.au

The raw data comes in the form of a spatial array of time series measured on the H-1 NF magnetic confinement experiment that studies a so-called stellarator design for a fusion reactor, i.e. it is a device to create, heat and confine a plasma. The plasma is confined in a roughly donut-shaped volume and subject to a number of instabilities, which potentially disrupt the confinement and may have detrimental effects on the device. Magnetic field probes are one the measurements that deliver information about these instabilities. Computationally, our approach consists of three steps: 1) First we generate a set of spatial basis functions using PCA. Then the time-dependent coefficients of the main basis functions are transformed with time-frequency transforms. The results are quantized and segmented in the time-frequency domain. 2) The second computational step consists of finding frequent pattern and association rules in the database of segments from step 1). A variant of the apriori algorithm is used for the search. 3) As the number of rules is large, we use a metric on the rules to determine clusters of similar rules. Other measures of interestingness that are based on the physical models of the systems are also employed. Together, these steps provide a powerful tool for investigation of causal relationships between different instabilities, and contribute to the global effort to identify indicators of, and ultimately prevent, disruptive instabilities in fusion reactors.

# Automated Registration for Augmenting Micro-CT 3D Images

Shane Latham  
Department of Applied Mathematics  
Australian National University, Australia  
Email: shane.latham@anu.edu.au

Micro-CT is a non-destructive means of creating 3D virtual models of an object of interest. With the advent of readily available commercial micro-CT systems, the analysis of tomographic images is rapidly gaining popularity for probing structure at the micro scale in a variety of applications. While the analysis of micro-CT images is able to characterise much of the geometrical information of a sample, X-ray attenuation alone is often insufficient for identifying the substances which comprise the sample. In addition, micro-CT is unable to resolve structure at sub-micron scales. To help overcome these micro-CT limitations, information gained from traditional microscopy techniques, can be combined with micro-CT data to provide a more complete description of the sample. In particular, we describe a method for automatically aligning (registering) Scanning Electron Microscope (SEM) 2D images of thin-sections with the corresponding region of the micro-CT 3D image. Our registration implementation is parallelised to take advantage of high-performance computational architectures and, to date, has been used to accurately align high-resolution SEM 2D images with micro-CT 3D images as large as 2048x2048x2048 voxels.

# Average and Deviation for Stochastic Fithugh-Nagumo System

Wei Wang  
USQ, Australia  
Email: wangw@usq.edu.au

Without a Lipschitz assumption, averaging equation is obtained by constructing an auxiliary process for a class stochastic partial differential equations with fast and slow time scales. Further the deviation between the original equations and the averaging equation is studied. It is proved by a martingale approach that the deviation is described by an Gaussian process.

# Changes in Flow and Wall Stresses through Arterial Constrictions Offset from the Vessel Centre

Charlene Chua  
Division of Biological Engineering  
Monash University, Australia  
Email: Charlene.Chua@eng.monash.edu.au

Arterial disease is the leading cause of death in the developed world, yet research into constrictions with an offset from the vessel centre has been limited. Blood flow through small, obstructed vessels is studied by computing time independent flows in tubes with sinusoidal constrictions, through a range of offsets. A high-order spectral element algorithm is employed to determine the extent of physiological flow characteristics such as recirculation zones and wall shear stress. Comparisons find that an increase in constriction offset gives rise to more intense shear stress and vorticity at the arterial wall. Moreover, these irregular flow conditions persist further downstream. Consistently, shear rate increases with Reynolds number and constriction offset. Streamwise vorticity increases linearly against constriction offset, with large variation at Reynolds numbers beyond 400 and 300 for axisymmetric and non-axisymmetric cases, respectively. Evidence of transition to three-dimensional flow is observed for the axisymmetric case. Vorticity perpendicular to the constriction geometry and shear rate both increase exponentially with constriction ratio. In the axisymmetric geometries, dissipation of the shear layers associated with downstream recirculation occurred more quickly; with larger constriction offsets, zones of high wall shear were found on the far wall downstream of the constriction, possibly causing degradation of the wall tissue.

# Characteristics of a Generalised Model of Host-Parasite Interactions

Steven Barry  
Pems South  
UNSW@ADFA, Australia  
Email: s.barry@adfa.edu.au

The dynamics of parasitic infection of ruminants have been modelled by considering the larval and adult stages of the parasite. The model involves two coupled linear ordinary differential equations, each of which has coefficients that are nonlinearly dependent on a third function that measures host immunity, thereby producing three nonlinear coupled ODEs. In previous work, the dependence of these coefficients on immunity has been assumed. However, we study the inverse problem of finding these parameters and their dependence on immunity using experimental data.

# Classification of Human Activity from Accelerometer Data

Garry Newsam  
DSTO, Australia  
Email: g.n.newsam@internode.on.net

DSTO has a long range research program on the use of light weight, wearable motion sensors for monitoring soldier activities in exercises and combat. A first step in this has been collection of tri-axial accelerometer data on subjects performing prescribed activities and analysis of this data to see if it supports detection and classification of these activities. The paper describes issues encountered and results obtained to date. On the plus side, a simple, linear time algorithm has reliably segmented the recorded time series. Starting with segmentation into single pixels, the algorithm sweeps upward: at each stage it merges the two neighbouring segments with the smallest value of a test statistic for the hypothesis that the segments come from the same Gaussian distribution. Setting thresholds on this statistic that give good segmentations is straightforward. Given a segmentation, computation of the power spectrum within each segment suffices for reliable classification into broad activity categories and detection of periodic motions. Accurate finer classifications, however, are not yet possible. The paper will also describe construction of new energy expenditure estimates from accelerometer data that are more accurate than those in previous papers. These take the form of minimum energy motions that are consistent with the accelerometer data. The results are regularisations with the unusual aspect that low frequencies are more heavily filtered than high.

# Computer Aided Optimisation of a Constant Shear-Rate Micro-Channel Contraction

Simon Higgins  
Monash University, Australia  
Email: Simon.Higgins@eng.monash.edu.au

A combination of spectral-element computational fluid dynamics (CFD) simulation and the Levenberg-Marquardt non-linear optimisation algorithm (LM) are used to optimise a micro-channel contraction. The CFD algorithm uses a spectral-element method for spatial discretisation and a third-order backward time integration scheme. The LM algorithm finds the local minimum of a function that is expressed as the sum of squares of nonlinear functions through an iterative process. The algorithm is adaptive as it controls its own damping which affects the solving approach. The primary criterion for the design of the micro-channel contraction is a constant shear-rate in the flow direction motivated by the need to study living cells in a uniform-shear environment. The LM algorithm is used to find the optimum contraction profile which minimises changes in the shear rate throughout the flow. This is achieved through successive iterations in which the flow field in the developing geometry is computed using the CFD package. The shear rates are then supplied to the LM solver, which calculates an improved estimate of the contraction geometry. From this data an improved mesh is constructed, and the iteration continues. Iteration concludes once minimum error conditions relating to the distribution of shear rate in the flow is achieved. This work has demonstrated a robust method for computationally aiding the design of micro fluidic channels.

# Controllability of a Class of Flexible Spacecraft with Nonlinear Terms

Fang Wang  
CAST, China  
Email: wffwj@163.com

Controllability has played a prominent role in the control theory and engineering, the concept of which was first proposed by Kalman in the early 1960s and has achieved sufficient advance. As to the rigid spacecraft, the global controllability is settled using differential geometry by Crouch (1984), where the controllability for the case when actuators are underactuated is also discussed. As to the more complicated flexible spacecraft, the linearized system model is employed with the property of the linear matrix-second-order system applied to prove its controllability. However, the actual model for flexible spacecraft is very complicated. The above researches are just focused on the simplified linear model for flexible spacecraft, with no consideration for the nonlinear term  $\dot{\omega}$ , where  $\omega$  is the angular velocity with respect to the principal axes of inertia;  $I$  is the inertial moment of the spacecraft without flexible deformation. Therefore, the contribution of the paper lies in the study of the controllability for the flexible nonlinear spacecraft using weakly positively Poisson stable theory and Lie-Poisson reduced dynamics knowledge. The main difficulty of the paper lies in proving the flexible spacecraft system satisfying the Lie algebra rank condition due to its complex nonlinear model. Without loss of generality, the system to be analyzed consists of one flexible appendage fixed at one end to the main body, which is capable of undergoing three-dimensional rotations.

# Direct Numerical Simulation of Turbulent Intermediate Froude Number Fountain Flow

Nicholas Williamson  
School of Aerospace, Mechanical Engineering  
University of Sydney, Australia  
Email: williamson@aeromech.usyd.edu.au

In this study the behavior of low Froude number turbulent fountain flow is examined with direct numerical simulation (DNS). Froude numbers from 0.5-3.0 have been simulated at a Reynolds number of 6676. The boundary condition of the turbulent fountain inflow has been generated using DNS of a periodic pipe flow simulation. At low Froude number, buoyancy forces are strong and the incoming flow penetrates only a short distance into the ambient domain before flowing radially out from the source. The mean flow is stabilised by buoyancy and the turbulent eddies in the flow dissipate quickly. At higher Froude number, the fountain penetrates a greater distance into the domain and the interaction between the rising fountain and the fountain fluid as it falls back towards the source is more important. This shear interaction increases entrainment between the two flows and the production of turbulent kinetic energy causing the fountain to become more unstable. The penetration height of the fountain is more unsteady and oscillatory compared to that at low Froude numbers.

# Discontinuous Galerkin Method for an Evolution Equation with Memory

William McLean  
School of Mathematics and Statistics  
University of New South Wales, Australia  
Email: w.mclean@unsw.edu.au

We consider an initial-boundary value problem for a fractional wave equation, and compute a piecewise-linear approximate solution, continuous in space but discontinuous in time. The error is globally of order  $k^2 + h^2 \log(1/k)$ , where  $h$  is the maximum diameter of the spatial elements and  $k$  is the maximum time step. The solution is superconvergent at the nodes of the time mesh, where the error is of order  $k^3 + h^2 \log(1/k)$ . To achieve these convergence rates, we must in general employ non-uniform time steps.

# Domain Decomposition Methods for Multiscale Elliptic PDEs

Ivan Graham  
Department of Mathematical Sciences  
University of Bath, UK  
Email: I.G.Graham@bath.ac.uk

In this talk we will discuss domain decomposition preconditioning for linear systems arising from finite element approximation of symmetric elliptic problems with highly variable coefficients. The work is motivated by problems arising in the computation of flow through heterogeneous media in 2D and 3D, in both the deterministic and stochastic cases. We will give condition number bounds which demonstrate how the subdomains and coarse space basis functions should be designed in order for the methods to be robust to both the heterogeneity of the media and the mesh parameters. In particular, we give a rigorous connection between low energy basis functions and robustness to heterogeneity. We also discuss the connections of the theory to the convergence of methods of AMG (algebraic multigrid) type, and give a number of computational illustrations of the theory. This is joint work with Rob Scheichl.

## Dynamic Hip Fracture Modelling

David Richards, John Arundell, Aaron Blicblau and Manmohan Singh  
Swinburne University of Technology, Australia  
Email: drichards@swin.edu.au

A treatment of Neck of Femur fractures is Internal Fixation using a Dynamic Hip Screw. This paper investigates the effect of the angle of such a Dynamic Hip Screw on the stresses developed under loading. The modelling is informed by an examination of Medicare Australia data which indicates that women aged 65 years or over are the primary recipients of an Internal Fixation of the Neck of Femur. Development of a series of Finite Element Models with incremental changes in angle allows determination of the stresses developed in use. Regression analysis of the data obtained from the Finite Element Analysis reveals a strong negative association between angle and stress.

## Effective diffusivities and time lag through multiple layers

Roslyn Hickson  
UNSW@ADFA, Australia  
Email: r.hickson@student.adfa.edu.au

We consider diffusion and reaction diffusion through multiple layers, with application to heat transport and plant spread. We derive some exact solutions, improving on recent existing work, and study ways to predict the time for transport across the layers (the time lag). We show the limitations of traditional methods of averaging the diffusivity, which are only applicable in the steady state and for numerous layers.

# Efficient Solvers for Incompressible Flows in Geosciences

Artak Amirbekyan  
Earth Systems Science Computational Center (ESSCC)  
University of Queensland, Australia  
Email: artak@uq.edu.au

Saddle point problems involving large systems of linear equations arise in wide variety of applications in computational science and engineering. A variety of solvers have been developed for this type of problems typically with specific applications in mind. In this paper we will focus on saddle point problems as they arise from incompressible flow problems in applications in geosciences. They are characterized through a spatially variable viscosity when modeling temperature dependencies (e.g. in Earth mantle convection models) or moving material interfaces (eg. in subduction zones simulation and numerical volcano models). In this paper we will give an overview on some of the iterative techniques that can be used and discuss suitable preconditioning techniques. We will discuss the implementation of the schemes using the python module `escript` and compare the efficiency of these schemes when applied to convection models on a parallel computer.

## Estimating Structural Equation Models Covariance Matrices Using Semi-Definite Programming.

Tania Prvan  
Department of Statistics  
Macquarie University, Australia  
Email: tprvan@efs.mq.edu.au

A new approach for estimating the covariance matrix associated with structural equation models will be presented. This covariance matrix can be expressed in terms of a vector of unknown parameters. The traditional method assumes the observations are distributed according to a multivariate normal distribution and uses maximum likelihood estimation to estimate the unknown parameters vector and hence the covariance matrix under the structural equation model being considered. The assumption of multivariate normality is not always realistic. Our new approach does not have any distributional assumptions. We obtain our estimate of the unknown parameters by minimizing the maximum absolute eigenvalue of the difference between the sample covariance matrix estimated from the data ignoring the structural equation model and the estimate of the covariance matrix based on the structural equation model. Semi-definite programming can be used to obtain the eigenvalues of a matrix if it can be written as a linear combination of non-negative definite matrices. We can do this for our structural equation model covariance matrix. The software `SeDuMi`, written in Matlab, can be used to do semi-definite optimization. Simulations have been conducted comparing our method with the traditional method described earlier. The distributions of the simulated data are deliberately not multivariate normally distributed.

# Estimating the Potential Predictability of West Australian Surface Temperature Using Monthly Data

Simon Grainger  
Bureau of Meteorology, Australia  
Email: S.Grainger@bom.gov.au

The seasonal mean of a climate variable can be considered to be a statistical random variable with two components: a 'slow' component which is potentially predictable at the long range (a season or more ahead), and an 'intraseasonal' component which is essentially unpredictable on this time scale. In this paper, an extension of a previous Analysis of Variance method is proposed which can deal with non-stationary data in transition seasons when estimating the 'intraseasonal' variability. By removing this from the total variability, an estimate for the 'slow' component, and hence the long range predictability of the seasonal mean is possible. The proposed method generates a system of equations relating the observed monthly moments to the 'intraseasonal' variability for each month and inter-monthly correlations. The system of equations is solved by a priori estimation of the inter-monthly correlations. For climate variables such as surface temperature, this is done by assuming that it can be modelled by a first-order auto-regressive process (i.e. red noise), and that the 'intraseasonal' variance changes linearly across a season. Once the inter-monthly correlations are obtained, the resulting system of equations can be solved by the numerical solution of one equation subject to constraint. The results from this method are investigated using monthly surface temperature data over Western Australia from 1951-2000.

## Estimation of Parameters for Two Spotted Spider Mite

Aspriha Chakraborty  
Swinburne University of Technology, Australia  
Email: achakraborty@swin.edu.au

This study concerns the interactions of the twospotted spider mite *Tetranychus urticae* and its predator *Phytoseiulus persimilis*. The logistic Lotka–Volterra predator–prey–taxis equations with diffusion and advection are solved numerically using two different response functions with one data set. The aim of this paper is to re-estimate parameters by using prey–taxis in the predator–prey system and to achieve successful biological control using prey–taxis. The method of the least squares is used to improve the goodness of fit of solutions to the field data. The stability of the point of equilibria are verified using Routh–Hurwitz's criteria.

## Exact Domain Walls and Their Stability

Zlatko Jovanoski  
School of Physical, Environmental and Mathematical  
UNSW@ADFA, Australia  
Email: z.jovanoski@adfa.edu.au

We obtain exact spatially periodic and localised domain wall solutions of a system of coupled nonlinear Schrodinger equations governing the propagation of light in a nonlinear medium. The solutions are facilitated through the use of Jacobi elliptic functions. These walls separate domains with different polarisation of light. Using both linear stability analysis and a beam propagation algorithm we demonstrate the stability of the domain walls.

# Existence, Uniqueness, and Approximation of Solutions to Dynamic Equations on Time Scales

Atiya Zaidi  
School of Mathematics and Statistics  
UNSW, Australia  
Email: a.zaidi@unsw.edu.au

An investigation on the existence, uniqueness and approximation of solutions to the dynamic initial value problem

$$\begin{aligned} \mathbf{x}^\delta &= \mathbf{f}(t, \mathbf{x}); \\ \mathbf{x}(a) &= \mathbf{A}. \end{aligned} \tag{3.2}$$

is presented. Here:  $t$  comes from a so-called "time scale"  $\mathbb{T}$ ;  $\mathbf{x}^\delta$  is the generalised derivative of a continuous function  $\mathbf{x} : \mathbb{T} \rightarrow \mathbb{R}^n$ . The system (3.2) describes dynamic processes which are continuous at one time and discrete at another in one model. The investigation is based on Banach's fixed point theorem and the introduction of a novel way of measuring distances in the time scale setting. The results show that a certain Lipschitz condition on  $\mathbf{f}$  not only guarantees the existence and uniqueness of solutions to (3.2), it also ensures the smoothness of the solution with respect to its initial value. This is an outcome of a joint work with Dr Chris Tisdell.

## Finite Element Methods for Nearly Incompressible Elasticity on Simplicial Meshes

Bishnu Lamichhane  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: Bishnu.Lamichhane@maths.anu.edu.au

It is well-known that the finite element approximations based on low order methods do not converge uniformly when applied to nearly incompressible elasticity. Many different methods are proposed to alleviate this problem. In the first part of the talk, we examine the classical Hu-Washizu mixed formulation for plane and three dimensional problems in linear elasticity with the emphasis on behavior in the incompressible limit. However, the Hu-Washizu formulation based on lowest order finite elements does not yield a stable formulation when the meshes consist of simplices. To tackle the problem of locking effect for simplicial meshes, we propose two novel methods based on primal and dual meshes and bases leading us again to the displacement-based formulations. These new approaches are easier to extend to non-linear elasticity than the approach based on the Hu-Washizu formulation. Numerical examples will be presented for all considered approaches.

# Flow Stability and Wall Shear Stress Profiles in Fusiform Aneurysms

Gregory Sheard

Department of Mechanical and Aerospace Engineering

Monash University, Australia

Email: Greg.Sheard@eng.monash.edu.au

Pulsatile flow through a tube with a sinusoidal dilation is computed to determine the wall shear stresses and flow dynamics under conditions representing blood flow through a human abdominal aortic aneurysm. Aneurysms manifest as local dilations of arteries which are prone to unexpected and lethal rupture. This study is motivated by research showing that aneurysm blood flow and wall shear stress contribute to the pathogenesis of aneurysms. A high-order spectral-element algorithm is employed to determine velocity and vorticity fields, and wall shear stresses, which are difficult to determine experimentally. A greater level of detail in the flow is revealed when compared to recent particle image velocimetry experiments. For both the mean and standard deviation of wall shear stress, minimum levels are found at the widest point of the aneurysm bulge, and maximum levels are recorded in the distal (downstream) region of the bulge. In an aneurysm with length and maximum diameter 2.9 and 1.9 times the artery diameter, respectively, peak instantaneous wall shear stress is 2.4 times greater than the peak wall shear stress recorded in a healthy vessel. A linear stability analysis predicts that human abdominal aortic aneurysm flows are unstable to non-axisymmetric disturbances.

## Fluid Flow Between Active Elastic Plates

Dmitry Strunin

University of Southern QLD, Australia

Email: strunin@usq.edu.au

We propose a model of channel flow between actively moving elastic walls as a framework for an autonomous model of blood flow in human arteries. The model is a dissipative partial differential equation with source, based on lubrication equations and some phenomenological principles controlling the movement of the walls. The PDE has similar structure to the equation we formulated earlier to simulate another active system - unstable front of solid-phase combustion.

# **Geometric Method for the 2-D Poisson Equation on an Irregular Domain with Mixed Boundary Conditions**

Ziad Jomaa  
School of Mathematics and Statistics  
University of Sydney, Australia  
Email: ziadj@maths.usyd.edu.au

We develop a 2-D algorithm for inverting the Poisson equation on an irregularly shaped domain, with mixed boundary conditions, using finite differences with the domain embedded in a rectangular Cartesian grid. We use both linear and quadratic boundary treatments and derive 1-D error expressions for both cases. The linear approach uses a 5-point formulation and is first-order accurate while the quadratic treatment uses a 9-point stencil and is second-order accurate. The key aspect of the quadratic treatment is the use of a suitably chosen directional derivative to find the second order accurate approximation to the normal derivative at the boundary.

## **Globally Stable Attitude Control of Underactuated Rigid Spacecraft**

Fang Wang  
CAST, China  
Email: wffwj@163.com

The underactuated spacecraft is characterized by the fact that the configuration of the actuators is incomplete, i.e., the actuators can't provide three independent control torques. The attitude control of underactuated spacecraft is very important for improving the reliability of the control system. Till now there have been many literatures about attitude control of underactuated spacecraft, however the best achievement till now is still locally stabilization with no globally stabilizing control law been reported as far as the authors know. Therefore the novelty of the paper lies in proposing a control method to solve the global stability problem of the underactuated rigid spacecraft. The idea is derived from the control method used in the practice. The details are as follows: first jet thrusters are used to stabilize the angular velocity of the rigid spacecraft, making the system angular momentum arrive at zero state; then flywheels are applied to achieve the global asymptotic stability of the system. In each step, the controller is constructed using the back-stepping method with the global stability analyzed based on the uniform ultimate boundedness lemma for the first step and Barbalats lemma and Lyapunov direct method for the second step.

## **Groundwater Response to Tidal forcing in Phreatic Aquifers**

Melanie Roberts  
School of Maths and Stats, UWA, Australia  
Email: melanie@maths.uwa.edu.au

Terrestrial groundwaters typically discharge into surface water bodies, and it is well understood that cyclic influences in surface water bodies can induce periodic behaviour within neighbouring aquifers. These behaviours have implications for a range of environmental concerns including salt-water intrusion and pollution migration. At short time scales, tidal forcing at phreatic aquifers are known to induce a periodic response in the watertable. We investigate the dynamics of the watertable response to tidal forcing across a sloping beach using a perturbation approach.

# Implementation of Outlet Boundary Conditions in Simulations of Unsteady Incompressible Flow

Michael Kirkpatrick  
School of AMME  
University of Sydney, Australia  
Email: m.kirkpatrick@usyd.edu.au

In numerical simulations of unsteady incompressible flow, mass conservation can be enforced using a fractional step method in which the momentum equations are solved in combination with a pressure or pressure correction equation. While there is an obvious way to implement most spatial boundary conditions commonly applied to these equations, the situation for so-called ‘outlet’ boundaries is less clear. Outlet boundaries must allow fluid to leave the domain with minimal effect on the upstream flow and, at the same time, ensure global conservation of mass. In previous work, we found that the outlet boundary condition implementations commonly used with lower order fractional step methods, such as the projection-1 and projection-2 methods, can cause the higher order projection-3 method to become unstable. In this paper we discuss the implementation of outlet boundary conditions in combination with fractional step methods, and investigate a number of alternative approaches.

## Interpolation on the Sphere: A Fast Solution Technique

Thanh Tran  
School of Mathematics and Statistics  
University of New South Wales, Australia  
Email: thanh.tran@unsw.edu.au

We present a fast solution technique for the problem of interpolation on the sphere, using radial basis functions and multiplicative Schwarz methods. Numerical experiments on relatively large scattered data point sets taken from MAGSAT satellite data will be presented.

## Intuitionistic Fuzzy Ideals Theory and Intuitionistic Fuzzy Local Functions

Ahmed Salama  
Faculty of Science, Port Said, Egypt  
Email: ahmed\_salama.2000@yahoo.com

In this paper we introduce the notion of intuitionistic fuzzy ideals which is considered as a generalization of fuzzy ideals studies, the important intuitionistic fuzzy ideals has been given. The concept of intuitionistic fuzzy local function is also introduced here by utilizing the  $\delta$ -neighborhood structure for a intuitionistic fuzzy topological space. These concepts are discussed with a view to find new intuitionistic fuzzy topology from the original one. The basic structure, especially a basis for such generated intuitionistic fuzzy topologies and several relations between different intuitionistic fuzzy ideals and intuitionistic fuzzy topologies are also studied here. Finally, several properties of all investigated new notions are discussed.

# **Kelvin Type Instabilities of Batchelor Vortex Pairs with Differing Circulations**

Christopher Butler  
Monash University, Australia  
Email: chris.butler@mac.com

The mutual co-existence of Batchelor vortices, and the resulting strain fields each vortex imposes on the other, can develop resonating Kelvin instabilities. These instabilities may lead to the accelerated dissipation of the vortices. The results presented are an analysis of a linearized growth rate of the Kelvin instabilities of the vortex pair. Here an axial velocity is imposed on the flow in addition to an asymmetry condition; that the vortices circulations are of different magnitudes. These flows improve current models of aircraft wakes, and will be relevant to aircraft maneuvers, such as during banking. These wakes, particularly from heavier aircraft, pose a significant risk to other aircraft, largely to the persistence resulting from slow dissipation rates, which occur without Kelvin-type instabilities. The study has focused on the Kelvin mode with the highest growth rate  $(-2,0,1)$  to give the clearest indications of effect on growth rate of the asymmetric condition. The study was performed numerically using a CFD package which, whose results have correlated well with both analytical and experimental work. The linear instability analysis, performed on a frozen base-flow was developed using a spectral-element simulation. Freezing the base-flow allows for the most efficient analysis of the instability growth rate.

## **Linear Stability Analysis of Counter-Rotating Unequal-Strength Batchelor Vortex Pairs**

Joine So  
Monash University, Australia  
Email: joine.so@eng.monash.edu.au

The instability of a counter-rotating unequal-strength Batchelor vortex pair is investigated numerically with a linear stability analysis technique. A high-order spectral-element method is employed to compute the time-dependent, incompressible flow in this investigation. The unequal-strength vortex pair is described by a ratio of the circulation strengths, and simulations are conducted at  $Re = 20000$ . Two Batchelor vortices are superimposed on a two-dimensional domain and evolved until they are deformed under strain, before the application of the stability analysis. The flow field is decomposed into a time-independent base flow and a perturbation field. The perturbation field is governed by the linearized Navier-Stokes equations providing insight into the global instability modes in the flow. An instability consistent with an elliptic instability is identified and described in the context of Kelvin modes. The predicted structure and growth rate of the instabilities are found to be dependent on the relative strength difference of the unequal-strength vortex pair and the axial wavelength of the instability of each mode. The branch modes of the instability can be recognized across a range of relative strength ratios. The structure and growth rate of the branch modes become less distinguishable when the difference in vortex strengths is further increased.

# Longitudinal Dispersion in a Horizontal Subsurface Flow Constructed Wetland: A Numerical Solution

Ercilia Sousa  
Department of Mathematics  
Coimbra University, Portugal  
Email: ecs@mat.uc.pt

We present a numerical solution for the dead zone model which describes the solute transport in a subsurface and horizontal flow constructed wetland. The dead zone model is a system of two mass balance equations for two conceptual areas: the main channel and the storage zone. The main channel is defined as that portion of the stream in which advection and dispersion are the dominant transport mechanisms. The storage zone is defined as the portion of the stream that contributes to transient storage. Within the main channel, solutes are transported downstream by advection and dispersion. Advection and dispersion are not included in the storage zones, where downstream transport is negligible. To determine the numerical solution of our problem we use finite difference schemes and we analyse its convergence through stability and accuracy. For the experimental results, the magnitude of the longitudinal dispersion and the extension of dead volumes is estimated for clean conditions and after a certain operating period. The results show a considerable amount of longitudinal dispersion through the bed, which was very strong near the feeding point, indicating the occurrence of mixing and significant presence of dead zones and short-circuiting.

# Mathematical Analysis of Microbial Depolymerization Processes of Xenobiotic Polymers

Masaji Watanabe  
Okayama University, Japan  
Email: watanabe@ems.okayama-u.ac.jp

The biodegradation is an important factor of environmental protection against undesirable accumulation of xenobiotic polymers. Microbial depolymerization processes fall into two types: exogenous type and endogenous type. In depolymerization processes of exogenous type, molecules lose their weight by separating monomer units from their terminals. Examples of polymers subject to exogenous-type depolymerization processes include polyethylene and polyethylene glycol. In depolymerization processes of endogenous type, molecules are split at arbitrary positions. Examples of polymers subject to endogenous-type depolymerization processes include polyvinyl alcohol and polylactic acid. In previous studies, mathematical models for those microbial depolymerization processes were proposed, experimental data were taken into analysis to determine degradation rates, and transitions of weight distribution were simulated. Here the mathematical analysis of microbial depolymerization of xenobiotic polymers. A mathematical model of microbial depolymerization process will be introduced, techniques to determine a degradation rate and to simulate the transition of weight distribution will be illustrated, and numerical results will be presented.

# **Model Turbulent Floods with the Smagorinski Large Eddy Closure**

Dmitry Strunin  
University of Southern QLD, Australia  
Email: strunin@usq.edu.au

Floods, tides and tsunamis are turbulent, yet conventional models are based upon depth averaging inviscid irrotational flow equations. We change the base of the average modelling to the Smagorinski large eddy closure for turbulence in order to appropriately match the underlying flow. The modelling allows for large changes in fluid depth to cater for extreme inundations. The key to analysis underlying the model is to choose surface and bed boundary conditions that accommodate constant shear as a nearly neutral mode. Analysis supported by slow manifold theory then constructs a model for the coupled dynamics of the fluid depth and the lateral mean velocity. The model resolves the internal turbulent shear in the flow and thus may be used in further work to rationally predict erosion and transport in turbulent floods.

# **Modelling Travelling Waves in Spatially Constrained Environments**

Farah Aini Abdullah  
School of Mathematical Sciences  
University Science Malaysia, Malaysia  
Email: robot77\_2000@yahoo.com

We will be looking at cell invasion modelling and our focus is the wavefront of the Neural Crest (NC) Cells in regard to Hirschsprung's Disease. This simulation model is performed using Fractional Differential Equations based on two basic cell functions. We simulate the model in one dimensional setting based on the Fractional Trapezoidal Scheme.

# **Modelling the Cryogenic Treatment of Warts**

Geoff Mercer  
Physical, Environmental and Mathematical Science  
UNSW@ADFA, Australia  
Email: g.mercer@adfa.edu.au

Cryotherapy is a commonly used and recommended treatment for warts. A variety of modes of application, recommended freeze times and interval between treatments are reported in the literature. Common recommendations are to create a 1-2mm halo of frozen tissue around the wart and freeze for 5-30 seconds. Larger freeze times are associated with increased risk of pain and blistering. Numerous texts suggest that the size of the wart determines the freeze time required without stating if this is the height, diameter or volume of the wart, or how the size and freeze time are related. There is wide variation in technique between clinicians applying the same mode of cryotherapy. To address this uncertainty in clinical practice a mathematical model is used to demonstrate the relationship between freezing time and tissue freezing zone for two commonly used cryogenes (liquid nitrogen spray and nitrous oxide probes).

# Multilevel Monte Carlo for Discontinuous Payoffs

Mike Giles  
Mathematical Institute  
Oxford University, UK  
Email: mike.giles@maths.ox.ac.uk

In previous research, I proved that for a set of coupled SDEs with a financial payoff function which is Lipschitz, the multilevel Monte Carlo method can achieve a r.m.s. accuracy of  $\varepsilon$  at a cost which is  $O(\varepsilon^2(\log \varepsilon)^2)$ . In this new work, I will show that (almost) the same complexity applies when the payoff function has discontinuities.

# Multivariate Density Estimation: A Sparse Grid Approach to Reducing the Curse of Dimensionality

Stephen Roberts  
Mathematical Sciences Institute  
Australian National University  
Email: stephen.roberts@anu.edu.au

With the recent growth in volume and complexity of available data has come a renewed interest in the problem of estimating a probability density function. Traditional methods however, fail to deal with the multivariate structure of this data and encounter the curse of dimensionality. Here we attempt to overcome this problem by applying the Sparse Grid technique, which has proven its ability to reduce the complexity of high dimensional problems in other areas. By using the intuitively simple histogram estimator as motivation, the problems of high dimensionality become apparent quickly. However, by considering this estimator as a finite element, grid based approach, the possibility of extending this technique using the Sparse Grids becomes clear. In particular, we demonstrate that the theoretical benefits of the Sparse Grids can be transferred to the density estimation problem. Using McDiarmid's exponential inequality, we show that the expected errors hold with high probability. We also present some numerical demonstrations of the performance of the Sparse Grid estimator on synthetic data.

# New Averaging Technique for Approximating Weighted Integrals

Grzegorz Wasilkowski  
Computer Science Department  
University of Kentucky, USA  
Email: greg@cs.uky.edu

We present a new averaging technique for studying the complexity of weighted multivariate integration problems. It allows us to conclude the existence of algorithms with the worst case errors bounded by  $O(n^{-1/2})$  for a wider class of problems than the techniques used so far. It also leads to more refined sufficient conditions for tractability of the multivariate integration problems, as well as a new class of randomized algorithms with errors bounded by  $O(n^{-1}\sqrt{\ln(\ln(n))})$  as opposed to typical bounds of  $O(n^{-1/2})$ . Joint work with L.Plaskota and Y.Zhao.

# Numerical Particle-like Solution of the Extended Hamilton-Jacobi Equation

Dmitry Strunin  
University of Southern QLD, Australia  
Email: strunin@usq.edu.au

In classical mechanics the Hamilton-Jacobi equation for a free particle has the property of reducing a perturbation of spatially uniform solution into a point. In the late 1970s Sivashinsky proposed an extension of the equation to the form of the now well-known Kuramoto-Sivashinsky equation under which a finite-size soliton is formed instead of a point. The soliton was put forward as a model of spatially extended elementary particle. However, this solution is unstable. Developing these ideas further, we propose another type of extension which ensures stability. We performed two-dimensional computational experiments demonstrating the process of soliton formation and analysed its dynamical structure.

## Numerical Simulation of Turbulent Flows

Linda Stals  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: stals@maths.anu.edu.au

The motivation behind this work is the solution of the Hasegawa-Wakatani equations that are used to model plasma flow. To design or predict the behavior of turbulent flows prolonged time series is required. The challenge is to find a numerical method that can allow long time steps without polluting the results with numerical instabilities. The primary focus of the talk is the solution of systems of non-linear ordinary differential using linear multistep methods. We will present a spectral based method applied to Hasegawa Wakatani equations.

## Numerical Solutions for Pseudodifferential Equations on the Sphere

Duong Pham  
School of Mathematics & Statistics  
University of New South Wales, Australia  
Email: z3238203@science.unsw.edu.au

In this talk we shall discuss the use of radial basis functions to find the collocation solution of pseudodifferential equations on the sphere. These equations arise from geodesy. Numerical experiments on relatively large scattered data point sets (taken from MAGSAT satellite data) will be presented.

# Numerical Study of Flow Generated in a Lake and Experiment Using GPS

Masaji Watanabe  
Okayama University  
Email: watanabe@ems.okayama-u.ac.jp

Currents generated in a lake are studied. A finite element method is applied to a system of partial differential equations governing the dynamics of flow. Experiments using a float equipped with a GPS unit, which called the GPS-float, are also conducted to validate numerical results. The driving force of the GPS-float is the fluid resistance on the pair of rectangular plates attached underneath the water surface. While the GPS-float travels on the surface, a GPS unit evaluates its position consecutively, and temporal and spatial data to track the float are transmitted to be recorded. On the other hand, the fluid resistance on the plates can be represented in terms of the velocity of flow. Once the fluid resistance is specified, the motion of the GPS-float can be simulated by solving its momentum equations, and a numerical result and an experimental result can be compared. The technique is used to determine the horizontal components of velocity and their vertical distribution. A technique to update depth data is also introduced. The depth data is measured with a sonar while the position is determined by a GPS unit. The three-dimensional data concerning the depth are used in the analysis of currents generated in a lake.

## On ODE Estimation Algorithms

Michael Osborne  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: mike.osborne@maths.anu.edu.au

The ODE estimation problem is concerned with differential equation models with solution trajectories that depend on the values of a finite number of parameters. It seeks to estimate these values using noisy observations made on the state variables during a particular solution trajectory. The two main approaches are the embedding and simultaneous methods. These formulate the estimation problem in distinctly different ways. This leads to equivalence questions which are not quite trivial, consistency questions which must take into account truncation errors, and solution methods with distinctly different computational properties. The Gauss-Newton method is favoured for optimisation problem associated with the embedding method. Is there an analogous method for the simultaneous approach?

## On Goedel's Proof

Stephen Boyce  
University of Sydney, Australia  
Email: stephen\_boyce@hotmail.com

This paper demonstrates that Goedel's proof may be modified to establish that Mendelson's first-order theory of Peano Arithmetic (S) is inconsistent. The result appears to be due to a defect in simple type theory rather than some peculiarity of S itself and poses a challenge for the view that every primitive recursive number-theoretic function is effectively computable.

# Oscillatory Combustion Waves in a Chain-Branching Reaction Model

Harvinder Sidhu

Email: harvinder.sidhu@adfa.edu.au

We investigate the properties of the travelling pre-mixed combustion waves in a model with two-step chain-branching reaction mechanism. These calculations were undertaken in the adiabatic limit and in one spatial dimension. We show that as the critical parameter is varied, there exist a critical value beyond which the combustion wave no longer travels with a single wave speed, but pulsates with a regular periodic pattern. We investigate the properties of the Hopf bifurcation (the point at which these pulsating wave emerges from the stable solution branch) and the pulsating combustion wave solutions. We also compare the solutions for our chain-branching model with its one-step counterpart and explain the similarities and differences between their behaviour.

# Parameterization of Subgrid-Scale Energy Injection in Oceanic Flows

Meelis Zidikheri

Theoretical Physics, RSPHysSE

Australian National University, Australia

Email: meelis.zidikheri@csiro.au

The phenomenology of quasi two-dimensional turbulence suggests that energy and enstrophy injected at some intermediate scales cascade in spectrally opposite directions: energy cascades towards the low wavenumbers (large scales) while enstrophy cascades towards the high wavenumbers (small scales). If a simulation is truncated at some smaller wavenumber, defining the resolved scales, then some form of parameterization is required to compensate for the absence of higher wavenumbers (the subgrid scales), which would either act as a net sink of enstrophy or as a net source of energy. In the former case, as occurs frequently in atmospheric simulations, some kind of dissipative term is usually employed, and there have been many studies to examine variants thereof. In the latter case, typical of oceanic simulations, this corresponds to a negative dissipation term. Such a term is, however, generally too numerically unstable to be of practical use. A solution to this problem is offered in this study in the form of a stochastic subgrid-scale parameterization scheme. Using quasigeostrophic models with typical oceanic parameters, it is shown that the scheme is able to maintain the resolved-scale spectra exceptionally well when the injection scale is not resolved. This work has implications for oceanic circulation modelling, where the deformation (injection) scale is too small to be adequately resolved.

# **Poisson-Nernst-Planck Theory and its Application to the Modelling of Neurons and their Environment**

Paul Nanninga  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: paul.nanninga@anu.edu.au

The Poisson-Nernst-Planck equations, describing the process of electrodiffusion, are applied to the neuron and its environment. Exact solutions of these equations, in time and 3-D, are found for systems containing 4 and more different valences, and any number of charge species, which can be used for model calibration. A simple computational model of ion channels is developed and incorporated into a fully calibrated numerical model that accurately solves the PNP-equations for an arbitrary configuration of membranes and ion channels in 3-D. The model allows the detailed study of electrochemical signalling in environments consisting of neurons and glial cells, without the computational cost of modelling the detailed structures and dynamics of ion channels. The model has the advantage over a molecular dynamics approach in that systems much larger than a single ion channel can be practically studied over much longer model runs. The model has the advantage over approaches based on cable theory (e.g. component models) in that it can take account of the 3-D time-dependent effect of electrochemical changes taking place in the extracellular fluid, as well as changes propagating along membranes.

## **Purging of Saline Fluid from a Cavity by an Overflow of Fresh Water on a Channel Bend.**

Natalie Gillam  
School of AMME  
Sydney University, Australia  
Email: n.gillam@usyd.edu.au

Purging of saline fluid from a cavity within a channel bend by an overflow of fresh water is investigated numerically and experimentally in this paper. A numerical simulation using a DNS fractional-step code is validated with a curved laboratory channel to determine the volume flux of saline density-stratified fluid purged from the cavity and the three-dimensional effects of the channel bend on the purging rate. The acceleration of the overflowing water through the bend as a result of centrifugal effects increases the near bed fluid velocity, and hence the rate of purging of saline fluid from within a channel bend is increased. This research is directly applicable to the purging of saline groundwater from the bases of rivers both within Australia and internationally, as the saline fluid is generally located within scour holes on the river bed found on river bends.

# QMC for Finance Beyond Black-Scholes

Jan Baldeaux

School of Mathematics and Statistics  
University of New South Wales, Australia  
Email: z3177364@science.unsw.edu.au

For the past decade, Quasi-Monte Carlo (QMC) Methods have been applied successfully to the pricing of financial derivatives in the Black-Scholes model. Empirically though, it has been observed that stock prices do jump and various models postulating that stock prices are driven by jump processes have consequently been proposed in the literature. Recently, QMC Methods have been used to price financial derivatives in some pure-jump models. However, jump-diffusion models have been given little attention from the point of view of QMC Methods. In this talk, we apply QMC Methods to a particular jump-diffusion model, namely the Kou model.

## Quantifying Parametric Uncertainty in Differential Equations

John Jakeman

Department of Mathematics  
Australian National University, Australia  
Email: john.jakeman@anu.edu.au

Differential equations are frequently used to model the behaviour of many complex systems. These systems are subject to a wide range of uncertainty in initial and boundary conditions, model coefficients, forcing terms and geometry. Uncertain input data is represented by random variables, which when substituted into the governing equations results in a stochastic system. Traditional Monte Carlo sampling is infeasible when model simulations require large amounts of computational time. An alternative method is to represent the uncertain quantities as a spectral expansion of orthogonal polynomials in terms of the uncertain random variables. These expansions can then be substituted into the governing equations and a Galerkin projection used to minimise the truncation error. This results in a system of coupled equations which can be solved using existing deterministic solvers. This approach is known as Generalised Polynomial Chaos (gPC) and exhibits exponential convergence for ‘smooth’ problems. A related approach known as Stochastic Collocation endeavours to combine the strengths of collocation and gPC methods. This approach determines the coefficients of the spectral expansion by interpolating a set of (uncoupled) deterministic solutions over the entire random space and uses numerical quadrature to evaluate the solution statistics. Here we present the gPC and the Stochastic Collocation when applied to ordinary differential equations exhibiting stable states and limit cycles.

# Resource Allocation and Component Scheduling Considerations for Parallel Coupled Systems

Jay Larson

Argonne National Laboratory, USA

Email: [larson@mcs.anl.gov](mailto:larson@mcs.anl.gov)

Simulation science is becoming increasingly complex due to the advent of coupled systems (e.g., coupled climate models). Parallel coupled multiphysics and multiscale models evolve through the execution of and mutual data exchange between numerous constituent codes. Teams developing these systems must decide how to assign resources to models (i.e., processors), and how to schedule constituent component execution. We review the two main strategies: serial composition, whereby constituent models each execute in turn on a single shared processor pool; and parallel composition, in which components each execute concurrently on their respective disjoint processor pools. We propose two other scheduling mechanisms: hybrid composition, which combines serial and parallel composition in nested form; and overlapping composition in which constituents may execute on partially intersecting processor pools. We develop a graphical notation for describing all of the above composition strategies. We also derive metrics based on constituent model scalability that can inform coupled model layout decisions. To demonstrate the utility of these ideas, we present examples from the field of coupled climate modeling.

## Revisiting the Transition to Unsteady Flow in an Open Cylinder with Rotating End Wall

Stuart Cogan

Monash University, Australia

Email: [stuart.cogan@eng.monash.edu.au](mailto:stuart.cogan@eng.monash.edu.au)

The flow driven by a rotating end wall in a cylindrical container has received much attention due to the development of stagnation points on the axis leading to a form of vortex breakdown. The spatio-temporal stability of such systems has been widely investigated numerically, theoretically and experimentally with Gelfgat et al. (2001) mapping the bifurcation structure in the Reynolds number - cylinder aspect ratio ( $Re$ ,  $H/R$ ) parameter space for the enclosed vessel and numerous publications confirming those findings (Marques and Lopez 2001; Thompson and Hourigan 2003). However, the flow in an open cylinder has received less attention with limited information available on the bifurcation properties of the open system. To the authors' knowledge only Lopez (1995) and Brons et al. (2001) have investigated the transition to unsteady flow in the open system with aspect ratio  $H/R=1.5$ . Thanks to renewed interest in the open vessel with  $H/R=1.5$  for the purposes of bioreactor design and optimisation (Dusting et al. 2006), the opportunity to revisit the stability characteristics of this system has arisen. Using highly resolved simulations of the axisymmetric Navier Stokes equations and a truncated Landau model we investigate the behaviour of the flow in the vicinity of the axisymmetric Hopf-type transition and report on the location and non-linear evolution characteristics of the bifurcation. Our results confirm and extend the findings of Brons et al. (2001) to fully define the transition.

# Scaled Boundary FEM Solution of Wave Diffraction by an Elliptic Cylinder

Longbin Tao  
Griffith School of Engineering  
Griffith University, Australia  
Email: l.tao@griffith.edu.au

In this paper, the scaled boundary finite-element method (SBFEM), a novel semi-analytical method, is modified to solve the wave interaction with an elliptic cylinder. By introducing a virtual circular cylinder surrounding the elliptic cylinder, the whole fluid domain is divided into one unbounded subdomain and several bounded subdomains. The corresponding boundary value problems in bounded and unbounded domains are solved by the SBFEM semi-analytically. Comparisons to the previous numerical solutions demonstrate the excellent computation accuracy and efficiency of the present SBFEM approach, as well as the benefit of not suffering from the difficulties of irregular frequency, which are often encountered by traditional boundary element method (BEM). The method can be extended to solve more complex wave-structure interaction problems resulting in direct engineering applications.

# Self-avoiding Random Walks on the Surface of a Sphere

Zbigniew, Stachurski  
Department of Engineering  
Australian National University, Australia  
Email: zbigniew.stachurski@anu.edu.au

Consider a randomly arranged cluster of touching spheres, comprising one inner sphere and  $k$  outer spheres, where  $4 \leq k \leq k_{\max}$ . The question is: how can the configuration of the randomly arranged cluster be described?

It will be proposed to use the concept of random walk as follows. Identify contact points between the inner and the outer spheres by radial vectors,  $R(j)$ , drawn from the centre of the inner spheres to the contact points on its surface. Then the configuration of the cluster can be described in terms of a vector polygon with vertices,  $R(j)$ , defined by the sum of the vectors, with an additional closing vector, zeta. The sum represents a chain of radial vectors which can be considered as a self-avoiding random walk restricted to the surface of the sphere.

# **Sensitivity of Block Entropy Based Complexity Metrics to Faulty Data**

Jay Larson  
Argonne National Laboratory, USA  
Email: [larson@mcs.anl.gov](mailto:larson@mcs.anl.gov)

One means of assessing complexity of timeseries data is to discretise it and study the resulting symbolic dynamics. Information-theoretic analyses are particularly useful for revealing structure in symbolic series. A number of complexity metrics exist that are derived from block entropy, in particular entropy rates of convergence identified by Crutchfield and Feldman, which have been shown to be skillful classifiers for periodic, random independent identically distributed, finite-order Markov, and infinitary processes. A key question is: How sensitive are these metrics to faulty data in the form of mis-assigned symbols? That is, if we change a fraction of the symbols  $f$ , will these block entropy metrics retain their skill, and how does this skill depend on  $f$ ? Results of ensemble Monte Carlo studies will be presented for both benchmark processes and coarse-grained observed precipitation data.

# **Simulation of Electromagnetic Interactions with Multiple Three Dimensional Particles**

Mahadevan Ganesh  
Department of Mathematical and Computer Sciences  
Colorado School of Mines, USA  
Email: [mganesh@mines.edu](mailto:mganesh@mines.edu)

Many physical phenomena occurring in atmospheric science, climatology, astronomy and medical science involve multiple electromagnetic scattering by an ensemble of non-spherical stochastic and deterministic particles such as ice crystals, atmospheric dust particles, and blood cells. We describe a fully discrete high-order algorithm for simulating low to medium frequency electromagnetic waves scattered by an ensemble of perfectly conducting three dimensional particles. A key component of our surface integral algorithm is the high-order tangential non-polynomial approximation of the surface current on each obstacle in the ensemble. We demonstrate the algorithm through parallel simulation of electromagnetic interactions with unique particles whose stochastic (and deterministic) description corresponds to computer models of ice crystals and dust particles (and red blood cells). This is a joint work with S. C. Hawkins.

# **Soliton Solutions for KdV Equation by Homotopy Analysis Method**

Hao Song  
Griffith University, Australia  
Email: h.song@griffith.edu.au

In this paper, the well-known KdV equation is solved by homotopy analysis method, an analytical, totally explicit technique. By choosing a proper auxiliary parameter, the new series solution converges very fast. The method provides us with a simple way to adjust the convergence region. Furthermore, a significant improvement of the convergence rate and region is achieved by applying Homotopy-Pad Approximants. The present method holds promise in providing soliton solutions for more complicated wave equations.

## **Solution of Large Sparse Singular Systems**

Ian Turner  
School of Mathematical Sciences  
QUT, Australia  
Email: i.turner@qut.edu.au

The complete solution of a large, sparse, linear system  $Ax = b$  requires an investigation of singularity and consistency. For small linear systems Gaussian elimination not only addresses these issues, it also provides a means to compute the solution. However for large systems, the elimination method can become impractical and for nonsingular systems, iterative methods based on Krylov subspace techniques are often preferred. Complications may arise with iterative methods when the matrix is singular, has many 'small' singular values or if the system is inconsistent. Solution by Null-space Approximation and Projection (SNAP) considers these problems as an integral part of the solution strategy by constructing an annihilator of the right hand side so that the solution then lies in the null space of the resulting matrix. We examine methods for constructing an approximate null space and present numerical case studies to illustrate the potential of our new method.

# Stochastic Subgrid Modelling for Atmospheric Large Eddy Simulations

Jorgen S. Frederiksen and Meelis J. Zidikher  
CSIRO Marine and Atmospheric, Australia  
Email: Jorgen.Frederiksen@csiro.au

Numerical and computational methods are presented for calculation of subgrid-scale parameterisations of unresolved dynamical processes needed for large eddy simulations (LES) of atmospheric flows. Long time simulations of atmospheric circulations in general circulation climate models are carried out at relatively coarse resolution corresponding to about 200 km. These LES require parameterisations of dynamical processes occurring at smaller scales through eddy viscosities and conductivities and stochastic backscatter parameterisations. Here, a stochastic modelling approach is presented to the subgrid modelling problem and applied to both barotropic and baroclinic atmospheric flows. The methodology consists of fitting a generalized Langevin equation, which takes into account memory effects of turbulent eddies, to the subgrid scales obtained from higher resolution direct numerical simulations (DNS) that are taken as the benchmarks. The parameterisations have a cusp behaviour at the cut-off wavenumber of the retained scales. When incorporated into the LES, the kinetic energy spectra and flow fields compare closely with the higher resolution DNS at the scales of the LES for both barotropic and baroclinic atmospheric flow. The method presented is generally applicable to the subgrid modelling problem.

## Surface Integral Equation Based T-Matrix Computations for Three Dimensional Acoustic Scattering

Stuart Hawkins  
School of Mathematics and Statistics  
UNSW, Australia  
Email: stuart.hawkins@unsw.edu.au

The acoustic scattering properties of an obstacle are completely described by its infinite acoustic T-matrix. The T-matrix is particularly useful when one is interested in analysing changes in sound wave propagation with respect to various changes in orientation or configuration of single or multiple scatterers. This is because the T-matrix is independent of the incoming wave directions and hence can be used to easily simulate the scattered sound waves (using substitution techniques), without the need to fully set up and solve each reconfigured system. However in practice one must use the truncated finite dimensional T-matrix, which is usually computed using the null field method. For acoustically large obstacles or highly nonspherical particles the null field method is numerically unstable. In this work we describe an efficient and stable method for computing the truncated T-matrix using a surface integral equation reformulation of the sound wave propagation problem and a high order acoustic surface scattering algorithm.

# Testing Mode-Coupling Theory Predictions Near and on the Freezing Line of a Simple Fluid

Alauddin Ahmed  
Swinburne University of Technology, Australia  
Email: aahmed@ict.swin.edu.au

The strain rate dependent power law exponents and coefficients of pressure and viscosity are calculated near and along the freezing line of Weeks-Chandler-Andersen (WCA) fluid applying nonequilibrium molecular dynamics (NEMD) simulation technique. The freezing line of the WCA system is calculated applying a novel algorithm which combines the elements of both equilibrium molecular dynamics (EMD) and NEMD methods. For pressure it is found that the standard mode-coupling theory value of the power law exponent  $= 3/2$  is limited to a very narrow region on the WCA freezing line and varies continuously between 1.7 to 1.9 as a function of freezing temperature and density, thus confirming its nonanalyticity. For the first time we report the freezing line viscosities of WCA system calculated through NEMD simulations. For each state point approaching the freezing line, a viscosity profile of the power law form is found to fit very well. Again in contrast to the standard mode-coupling theory value of 0.5, the viscosity exponent can have values between 0.2 and 2 in the dense liquid phase. We have found that for isotherm 1.15, densities below 0.88, power law exponent is a linear function of temperature and the coefficients diverge rapidly and faster than their liquid state counterparts following stretched exponential form. In the vicinity of freezing densities the power law behavior is failed to represent the predicted behavior.

# The Application of the Aerodynamic Reciprocity Principle in Turbulent Flows Past Objects

Tracie Barber  
UNSW, Australia  
Email: t.barber@unsw.edu.au

The principle of aerodynamic reciprocity established by Da Vinci in the 16th century is invoked whenever it is asserted that aerodynamic forces are the same whether an object is moving in a stationary air or moving air flows past the same stationary object. A 2D numerical analysis has been conducted to determine the validity of this principle when applied to a body moving through a turbulent flow as in a wind tunnel or moving through a stationary fluid as in a towing tank. The feasibility of a moving airfoil simulation when implemented in a commercial CFD code was first confirmed. Then, two simulations were performed, one with a moving airfoil in a still fluid and the other with a stationary airfoil in a fluid moving with the same velocity as the moving airfoil. Initially a laminar simulation was used and a comparison made between lift and drag forces, flow fields, and convergence efficiency. The exact equivalence between the moving and stationary airfoil simulations was confirmed when using the 2nd order upwind discretization scheme, laminar steady state formulation. However, when turbulence was simulated, differences emerged in both the lift and drag forces, depending on whether the airfoil or the fluid was stationary (and therefore, whether free-stream turbulence was introduced at the inlet). Further, there were significant differences in the details of the flow between the two cases, in particular in the turbulence energy distribution around the airfoil.

# **The Convergence of the Immersed Interface Method for Two Channels Dissipation Model with Discontinue Constants Velocity**

Sumardi Sumardi and Soeparna Darmawijaya and Lina Aryati  
Dept. of Mathematics, Gadjah Mada University  
Indonesian Mathematics Society, Indonesia  
Email: mas\_mardi@yahoo.com

The Immersed Interface Method can approximate the exact solution one dimensional two channels dissipation model in heterogeneous media. The method obtained two kinds continuous solution that: density and flux. The idea of the standard scheme Lax-Wendroff is used for regular grids, but the immersed interface methods is applied on a set of modified values deduced from numerical values and from jump conditions on interfaces. Numerical examples show that we can compute solutions to these equations with second order accuracy. The purpose of this paper is to investigate the convergence of the immersed interface method for two channels dissipation model with discontinue constants velocity. We analyze the stability using generalized Von Neumann analysis and the convergence of the method using Lax Equivalence Theorem.

## **The Rheological Inverse Problem of Interconversion between Relaxation to Creep**

Robert S. (Bob) Anderssen  
CSIRO Maths and Stats, Australia  
Email: Bob.anderssen@csiro.au

Recent work by Davies, de Hoog and anderssen have resolved theoretically that the interconversion from relaxation to creep is stable, while that from creep to relaxation can be unstable. Until this work, the result was only known numerically and consequently, the role of the numerical method as the source of the instability could not be rule out. This extends the work on this problem reported at CTAC06.

# **The Total Quasi-Steady State Assumption: Its Justification by Singular Perturbation Theory and its Application to the Chemical Master Equation**

Chin Foon Khoo and Markus Hegland  
Australian National University, Australia  
Email: khoo@maths.anu.edu.au

Deterministic models of enzymatic reaction based on the quasi-steady state assumption (QSSA) and total quasi-steady state assumption (tQSSA) have been used successively in the past. This is surprising as the QSSA and tQSSA can neither be verified mathematically nor by experiment for most cases of interest. Here, different from the work of Schnell and Maini (2001) before, we discuss an approach using singular perturbation theory to justify the approximation obtained by tQSSA by referring to the idea of Segel and Slemrod(1989), which applies perturbation analysis on the QSSA. In addition, we extend the application of tQSSA to the stochastic model to deal with stiff differential equations originating from the chemical master equation (CME). Keywords: tQSSA, singular perturbation method, CME

## **The Validity of Axisymmetric Assumptions When Investigating Pulsatile Biological Flows**

R. Aidan Jamison  
Division of Biological Engineering  
Monash University Clayton, Australia  
Email: robert.jamison@eng.monash.edu.au

The use of computational fluid dynamics in investigating biological flows is increasing in popularity due to its ability to define the flow throughout the entire domain, a limiting factor for experimental work. A common assumption across prior studies is that both the geometry and the flow field through an aneurysm is axisymmetric, however investigations into non-biological flows have seen that even with an axisymmetric geometry non-axisymmetric flow is able to develop. Idealised geometries are used to investigate these biological flows as it simplifies the model to enable an improved understanding of the effect geometry has on the flow. Additionally this simplification allows the implementation of a computationally cheaper axisymmetric code. The current study tests this axisymmetric assumption by applying Floquet stability analysis to predict the conditions under which an axisymmetric aneurysmal flow is unstable to non-axisymmetric instabilities. A non-dimensionalised pulsing frequency was input upstream and a Reynolds number range relevant to aneurysms in large arteries examined. Non-axisymmetric flow was observed to develop for a significant range of these conditions.

# Time-Fractional Distributed Order Symmetric Space-Fractional Diffusion Equation

Qianqian Yang  
School of Mathematical Sciences  
Queensland University of Technology, Australia  
Email: q.yang@qut.edu.au

In this paper, one analytical and two practical numerical solution strategies are provided to solve a time-fractional distributed order symmetric space-fractional diffusion equations (TFDO-SSFDE) under homogeneous Dirichlet boundary conditions. Firstly, a method of separating variables is effectively implemented to express the analytical solution of the TFDO-SSFDE in terms of the Mittag-Leffler function. Secondly, we develop two numerical methods to deal with the symmetric space-fractional derivatives; namely, the Shifted Grunwald method, and the matrix transform method. To discretize the Caputo time fractional derivative, a finite difference approximation is adopted. Finally, numerical examples are presented which demonstrate the effectiveness of the methods and confirm the theoretical claims.

## Tractability of Multivariate Approximation: Smoothness Sometimes Hurts

Henryk Wozniakowski  
Department of Computer Science  
Columbia University, USA  
Email: henryk@cs.columbia.edu

Folk wisdom tells us that as the smoothness of a problem increases, the problem becomes easier. We provide a counterexample to this folk-belief. It will be done for multivariate approximation over a weighted unanchored Sobolev space having smoothness  $m \geq 1$ . We prove that for  $d$ -variate functions we need at least  $m^d$  function values or linear functionals to guarantee that the worst case error is less than 1. Hence, for  $m \geq 2$  the problem suffers from the curse of dimensionality. On the other hand, for  $m = 1$  the curse is not present under properly decaying weights. The talk is based on a joint paper with A. G. Werschulz.

# **Using FCM to Analyze the Customer Satisfaction in an Iranian Automotive Company**

Somayeh Alizadeh  
Iran  
Email: sima.alizadeh@yahoo.com

There are numerous factors in production and sales systems which affect not only each other but also customer satisfaction and company profitability. Identifying and ranking critical factors of these systems permits managers to obtain a better understanding of these systems and increase the customer satisfaction. A good way of identifying these relationships is using Fuzzy Cognitive Map. In this paper, two novel techniques are proposed. The first one is a method for learning FCM based on historical data by using some meta-heuristic methods and the second one is a method for ranking the essential components based on their cause and effect behaviors. Implementation of the two proposed methods has demonstrated by using real data from production and sales systems in an Iranian automotive company.

# **Using Memetic Algorithm to Learn FCM in Modeling Agile NPD Process**

Somayeh Alizadeh  
Iran  
Email: sima.alizadeh@yahoo.com

The new product development process is an integrated process and all the stages of the NPD process are related to each other. All main factors which affect on the agile NPD process are also related to each other. Identification of critical factors of agile NPD permits the managers to obtain a better understanding of issues surrounding the agile NPD process. A good way of identifying the relationships between the agile NPD processes in manufacturing companies is applying Fuzzy Cognitive Map. This FCM shows the relation between all main items of agile NPD process and help managers to extract a good view of this process and improve their decision quality. In this paper, a novel learning model is proposed to learn FCM by using Memetic Algorithm (MA) from related data. The efficiency of the proposed model is shown via comparison of its results with Genetic Algorithm (GA). Implementation of this proposed model has demonstrated via real data of the agile NPD process in Iranian Manufacturing enterprises.

# Using Scalapack to Parallelize Optimization on the Sphere

Paul Leopardi  
Mathematical Sciences Institute  
Australian National University, Australia  
Email: paul.leopardi@maths.anu.edu.au

The sphere optimization program SPHOPT optimizes the value of a determinant as a function of a finite number of points on a sphere. It was written as a sequential program using LAPACK, and was converted to use ScaLAPACK, mainly to overcome memory limitations. This talk describes the principles needed to convert LAPACK programs to ScaLAPACK, and how they were applied to SPHOPT. In particular the talk will describe a compressed block cyclic storage scheme to store two symmetric matrices in little more than the storage needed for one matrix. Scalability results on the APAC SC and AC will also be discussed. This is joint work with Rob Womersley, UNSW.

# Visual Cortex Mapping by Conjugate Gradients

David Smith  
Queensland Brain Institute  
University of Queensland, Australia  
Email: dherschelsm@yahoo.com

Neurons in the cerebral area known as primary visual cortex respond selectively to different stimulus attributes such as position and orientation. Associated mapping calculations seek these preferences on a cortex lattice, given a set of visual stimuli, much like a fluid flow calculation seeks pressures or velocities on a mesh. Vortex-like structures known as pinwheels are present in the orientation preference map, and previous studies based on a dynamical systems approach have demonstrated an intimate link between the developmental phenomenon of pinwheel annihilation and another visual property known as ocular dominance. Ocular dominance segregation was shown to act as a pinwheel annihilation suppression agent, which explained a number of observed inter-species differences. Without ocular dominance segregation, copious pinwheel annihilation generates a distinct pattern of large stripe-like iso-orientation domains, with local plane wave structure and sparse pinwheel density. This talk will describe an alternative route to these striking patterns, via the application of conjugate gradient iteration to a certain objective function related to the dynamical systems approach. Achieving sufficiently low function values is not a simple matter, demanding careful consideration of the search direction update and line search parameters. Convergence and sensitivity issues will be examined, comparing iteration trajectories, and showing the signatures of key evolution mechanisms.

# Visual Cortex Mapping by Conjugate Gradients

John Belward and Ian Turner  
QUT, Australia  
Email: john.belward@qcscm.com

We present an error analysis and results of a numerical investigation for least squares estimates of gradients. These are strategies for approximating the gradients of functions which are known only as a set of scattered data values. In previous work [1] we have observed second order accuracy with each and we have shown that although both strategies appear different, they produce the same least squares error. The method amounts to setting up a least squares problem using a Taylor expansion. Intuition suggests that the order of magnitude of the error will be that of the remainder term in the Taylor expansion. A theoretical analysis confirms this, but a coefficient in the error bound is proportional to the inverse of the smallest singular value of the least squares matrix. We report on numerical experiments which compare the observed errors and theoretical bounds. The error bounds are often pessimistic by several orders of magnitude. The circumstances in which this takes place are examined. They lead to an empirical correction of the theoretical error bounds and an indication of how this idea can be supported by a rigorous argument.

1. J. A. Belward, I. W. Turner, and M. Ilic. On derivative estimation and the solution of least squares problems. To appear in J.C.A.M.
2. J.A. Belward, I.W.Turner and M.N. Oqielat. A Hybrid Clough-Tocher Radial Basis Function Method for Modelling Leaf Surfaces. <http://mssanz.org.au/MODSIM07>

# Index

- Abdullah, Farah Aini, 33  
Ahmed, Alauddin, 45  
Alizadeh, Somayeh, 49  
Amirbekyan, Artak, 25  
Anderssen, Robert S. (Bob), 46  
Andrew, Alan, 15  
Ang, Keng Cheng, 11
- Baldeaux, Jan, 39  
Barber, Tracie, 45  
Barry, Steven, 16, 21  
Belward, John, 51  
Boyce, Stephen, 36  
Brenner, Susanne, 4  
Butler, Christopher, 31
- Chakraborty, Aspriha, 26  
Chua, Charlene, 20  
Cogan, Stuart, 40
- Detering, Frank, 19
- Forbes, Larry, 4  
Frederiksen, Carsten, 10  
Frederiksen, Jorgen, 44
- Ganesh, Mahadevan, 42  
Giles, Mike, 34  
Gillam, Natalie, 38  
Graham, Ivan, 24  
Grainger, Simon, 11, 26
- Hawkins, Stuart, 10, 44  
Hegland, Markus, 18  
Hickson, Roslyn, 24  
Higgins, Simon, 22
- Jakeman, John, 39  
Jamison, R. Aidan, 47  
Jomaa, Ziad, 29  
Jovanoski, Zlatko, 26
- Keyes, David, 5  
Khoo, Chin Foon, 47  
Kirkpatrick, Michael, 30  
Kuroiwa, Nao, 15
- Lamichhane, Bishnu, 27
- Larson, Jay, 40, 42  
Latham, Shane, 19  
Le Gia, Quoc Thong, 13  
Leopardi, Paul, 50  
Ly, Eddie, 17
- Mclean, William, 23  
Mercer, Geoff, 33  
Moroney, Timothy, 14  
Mustapha, Kassem, 12
- Nanninga, Paul, 38  
Newsam, Garry, 21
- OKane, Terence, 16  
Osborne, Michael, 36
- Pennifold, Richard, 18  
Petzold, Linda, 6  
Pham, Duong, 35  
Prvan, Tania, 25
- Richards, David, 24  
Roberts, Melanie, 29  
Roberts, Stephen, 34  
Rowe, Martin, 14  
Ruede, Ulrich, 6
- Salama, Ahmed, 30  
Sampson, Joe, 12  
Sheard, Gregory, 28  
Sidhu, Harvinder, 37  
Simpson, Daniel, 13  
Sinha, Rajen, 12  
Sloan, Ian, 7  
Smith, David, 50  
So, Joine, 31  
Song, Hao, 43  
Sousa, Ercilia, 32  
Stachurski, Zbigniew, 41  
Stals, Linda, 35  
Stephan, Ernst, 8  
Strunin, Dmitry, 28, 33, 35  
Sumardi, Sumardi, 46
- Tao, Longbin, 41  
Towers, Isaac, 17

Tran, Thanh, 30

Turner, Ian, 43

Wang, Fang, 22, 29

Wang, Wei, 20

Wasilkowski, Grzegorz, 34

Watanabe, Masaji, 32, 36

Williamson, Nicholas, 23

Wozniakowski, Henryk, 48

Yang, Qianqian, 48

Zaidi, Atiya, 27

Zidikheri, Meelis, 37