Warwick
Mathematics Research Centre

# Warwick EPSRC Symposium 2008/09
# Challenges in Scientific Computing
# Organiser: Andrew Stuart

**Tuesday 30 June - Friday 3 July 2009** **Capstone Conference**

**Organiser: Andrew Stuart**

## Plenary Talks in Lecture Room MS.01 Ground Floor
## Minisymposia in Lecture Rooms MS.04, MS.05, B3.02 are on the 3rd Floor
## all are in the Zeeman Building

## Tuesday 30 June 2009

*Chair: Andrew Stuart*

09:15–10:00 Plenary **Anna-Karin Tornberg** (Stockholm) *Model reduction for efficient simulation of fiber suspensions*

10:00–10:45 Plenary **Mike Shelley** (Courant) *Microscale instability and mixing in driven and active complex fluids*

10:45–11:30 Tea and Coffee in The Street

11:30–12:15 Plenary **Darren Wilkinson** (Newcastle) *Stochastic modelling and Bayesian inference for biochemical network dynamics*

12:15–13:00 Plenary **TBA**

13:00–14:30 Lunch in Room A0.05 off The Street

14:30–15:30 ***Minisymposia***

Room MS.04 Organiser: **Jared Tanner** *Sparse approximation and compressed sensing*

Room MS.05 Organiser: **Omiros Papaspiliopoulos** *Stochastic modelling and computer-intensive inference in biology*

Room B3.02 Organiser: **Steve Coombes** *Mathematical neuroscience*

15:30–16:15 Tea and Coffee in The Street

16:15–17:15 ***Minisymposia***

Room MS.04 Organiser: **Jared Tanner** *Sparse approximation and compressed sensing*

Room MS.05 Organiser: **Omiros Papaspiliopoulos** *Stochastic modelling and computer-intensive inference in biology*

Room B3.02 Organiser: **Steve Coombes** *Mathematical neuroscience*

## Wednesday 1 July 2009

*Chair: Ben Leimkuhler*

09:15–10:00 Plenary **Tony LeLievre** (ENPC, Paris) *Sampling problems in molecular dynamics*

10:00–10:45 Plenary **Rupert Klein** (Berlin) *Challenges in modelling and computing planetary scale atmospheric flows at high resolution*

10:45–11:30 Tea and Coffee in The Street

*Chair: Nancy Nichols*

11:30–12:15 Plenary **Roland Freund** (UC Davis) *Krylov subspace-based dimension reduction of large-scale linear dynamical systems*

12:15–13:00 Plenary **Michael Overton** (New York) *Characterization and construction of the nearest defective matrix via coalescence of pseudospectra*

13:00–14:30 Lunch in Room A0.05 off The Street

14:30–15:30 ***Minisymposia***

Room MS.04 Organiser: **Nancy Nichols** *Model reduction*
Room MS.05 Organiser: **Colin Cotter** *Lagrangian structure, Lagrangian data*
Room B3.02 Organiser: **Ben Leimkuhler** *Molecular dynamics in and out of equilibrium*

15:30–16:15 Tea and Coffee in The Street

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## Thursday 2 July 2009

***Chair: Michael Allen***

09:15–10:00 Plenary **Daan Frenkel** (Cambridge) *Polymer simulations and Bayesian data analysis*

10:00–10:45 Plenary **Eric Vanden Eijnden** (Courant) *Theory and modeling of reactive events*

10:45–11:30 Tea and Coffee in The Street

***Chair: Endre Suli***

11:30–12:15 Plenary **Franco Brezzi** (Pavia) *Recent perspectives on discontinuous Galerkin methods*

12:15–13:00 Plenary **Tom Hou** (CalTech) *The interplay between computation and analysis in the study of 3D incompressible flows*

13:00–14:30 Lunch in Room A0.05 off The Street

14:30–15:30 ***Minisymposia***

Room MS.04 Organiser: **Mike Allen** *Future directions in molecular simulation*
Room MS.05 Organiser: **Coralia Cartis** *Optimization*
Room B3.02 Organiser: **Endre Suli** *Numerical analysis of nonlinear evolution equations*

15:30–16:15 Tea and Coffee in The Street

16:15–17:15 ***Minisymposia***

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Room B3.02 Organiser: **Endre Suli** *Numerical analysis of nonlinear evolution equations*

## Friday 3 July 2009

***Chair: Charlie Elliott***

09:15–10:00 Plenary **Emmanuel Candes** (CalTech) *Fast algorithms for the computation of oscillatory integrals*

10:00–11:00 ***Minsymposia***

Room MS.04 Organiser: **Greg Pavliotis** *Numerical methods for multiscale stochastic systems*
Room MS.05 Organiser: **Jason Frank** *Computational methods for geophysical flows*
Room B3.02 Organiser: **Charlie Elliott** *Computational methods for interfaces and surfaces*

11:00–11:45 Tea and Coffee in The Street

11:45–12:45 ***Minsymposia***

Room MS.04 Organiser: **Greg Pavliotis** *Numerical methods for multiscale stochastic systems*
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12:45–14:00 Lunch in Room A0.05 off The Street

*If you have any questions during the workshop please see either Hazel Higgens or Yvonne Collins in Room B1.37 which is opposite the Common Room*

Tuesday 30 June – Friday 3 July 2009

# Capstone Conference • Abstract of Plenary Talks

## All Plenary Talks are in MS.01 • Zeeman Building

**Franco Brezzi** (IMATI-CNR and IUSS-Pavia) ***Recent perspectives on Discontinuous Galerkin methods***

Roughly speaking, Discontinuous Galerkin methods aim at finding the approximate solution of a boundary value problem for PDE looking, a priori, among piecewise polynomial functions that might be discontinuous in the passage from one element to the neighboring one.

Recently DG methods have been applied to several types of problems (from the "original" conservation laws to continuous mechanics to electromagnetic problems) and analyzed from several perspectives (from hybridizable methods to weighted residuals).

The talk will start with a brief glance at the whole panorama, and then concentrate on pros and cons of the least squares approach in several applications.

**Emmanuel Candes** (CalTech) ***Fast algorithms for the computation of oscillatory integrals***

This talk introduces a novel multiscale algorithm for the numerical evaluation of Fourier integral operators whose overall structure follows that of the butterfly algorithm. This is of interest for such fundamental computations are connected with the problem of finding numerical solutions to wave equations, and also frequently arise in many applications including reflection seismology, curvilinear tomography and others. This algorithm is accurate, is highly efficient in terms of memory requirement, and runs in O(N log N) flops where N is the number of input/output components, thus enjoying near-optimal computational complexity.

This is joint work with Laurent Demanet and Lexing Ying.

**Roland Freund** (UC Davis) ***Krylov subspace-based dimension reduction of large-scale linear dynamical systems***

Krylov subspace methods can be used to generate Pade approximants of the transfer functions of linear dynamical systems. Although this Krylov-Pade connection has been known for a long time, somewhat surprisingly, it was not until the 1990s that this connection was exploited to devise practical numerical procedures for dimension reduction of large-scale linear dynamical systems.

In this talk, we first describe a problem arising in the simulation of electronic circuits that had triggered the interest in Krylov subspace-based dimension reduction in the 1990s. We then present an overview of the current state-of-the art of this class of dimension reduction algorithms. In particular, we focus on recent advances in structure-preserving reduction techniques. Finally, we describe a number of open problems in Krylov subspace-based dimension reduction.

**Tom Hou** (CalTech) ***The interplay between computation and analysis in the study of 3D incompressible flows***

Whether the 3D incompressible Navier-Stokes equations can develop a finite time singularity from smooth initial data is one of the most challenging problems for both computation and analysis. We review some recent theoretical and computational studies of the 3D Euler equations which show that there is a subtle dynamic depletion of nonlinear vortex stretching due to local geometric regularity of vortex filaments. The local geometric regularity of vortex filaments can lead to tremendous cancellation of nonlinear vortex stretching. We also investigate the stabilizing effect of convection in 3D incompressible Euler and Navier-Stokes equations. The convection term is the main source of nonlinearity for these equations. It is often considered destabilizing although it conserves energy due to the incompressibility condition. Here we reveal a surprising nonlinear stabilizing effect that the convection term plays in regularizing the solution. Finally, we present a new class of solutions for the 3D Euler and Navier-Stokes equations, which exhibit very interesting dynamic growth property. By exploiting the special structure of the solution and the cancellation between the convection term and the vortex stretching term, we prove nonlinear stability and the global regularity of this class of solutions.

**Rupert Klein** (Berlin) ***Challenges in modelling and computing planetary scale atmospheric flows at high resolution***

Current production General Circulation Models (GCMs) for global atmospheric flow simulations are based on the Hydrostatic Primitive Equations (HPEs). These result from the full three-dimensional compressible flow equations in the limit of large horizontal-to-vertical scale ratios. While this asymptotic limit suppresses vertically propagating sound waves, it does support long-wave horizontally travelling acoustic modes, which are called "Lamb waves" and are considered important.

In contrast, current computational simulations of small-scale atmospheric processes, such as cloud formation, local storms, or pollutant transport on city-scales, are based on analogues of the classical incompressible flow equations, i.e., they are "sound-proof".

Modern high-performance computing hardware is beginning to allow atmospheric flow modellers to use grids with horizontal spacing in the range of merely a few kilometres. At such high resolution, the hydrostatic approximation breaks down, and one enters the scale range of sound-proof model applications.

In this lecture, I will elucidate why simply resorting to solving the full compressible flow equations without approximation on high-resolution grids is not as straight- forward as it may seem, I will explain numerical techniques designed to address the ensuing issues, and I will summarize recently proposed sets of multiscale model equations that are designed to capture both regimes at the continuum level while maintaining the advantages of the established single-scale equation sets.

**T. LeLievre** (ENPS) ***Sampling problems in molecular dynamics***

One aim of molecular dynamics is to compute some macroscopic quantities from microscopic models, through means of some relevant observables in an appropriate thermodynamic ensemble. These calculations are typically difficult because the measure to sample is highly metastable, which makes classical Markov Chain Monte Carlo algorithms very slow to converge. We review some classical methods which are used in molecular dynamics to deal with this problem, with an emphasis on adaptive importance sampling methods.Applications of the method to other field (such as Bayesian statistics) are mentioned.

**Michael Overton** (New York) ***Characterization and construction of the nearest defective matrix via coalescence of pseudospectra*** (coauthors are R. Alam, S. Bora and R. Byers)

Let $w(A)$ be the distance from a matrix $A$ to the set of defective matrices, using either the 2-norm or the Frobenius norm, and let $c(A)$ be the supremum of all $\varepsilon$ with the property that the open $\varepsilon$-pseudospectrum of $A$ has $n$ distinct components in the complex plane. Demmel and Wilkinson independently observed in the early 1980s that $w(A) \geq c(A)$, and equality was

established for the 2-norm by Alam and Bora in 2005. We give new results on the geometry of the pseudospectrum near points where coalescence of the components occurs, characterizing such points as the lowest generalized saddle point of the smallest singular value of $A - zI$ over $z \in C$ . One consequence is that $w(A) = c(A)$ for the Frobenius norm too, and another is the perhaps surprising result that the minimal distance is attained by a defective matrix in all cases. Our results suggest a new computational approach to approximating the nearest defective matrix; numerical experiments that support the usefulness of this idea are given. In addition we present several open questions and conjectures.

**Mike Shelley** (Courant) ***Microscale instability and mixing in driven and active complex fluids***

Complex fluids are fluids whose suspended microstructure feeds back and influences the macroscopic flow. A well-known example is a polymer suspension and a novel one is a bacterial bath wherein many swimming micro-organisms interact with each other through the surrounding fluid. In either case, these systems can display very rich dynamics even at system sizes where inertia is negligible, and both systems have important applications to micro-fluidic mixing and transport. They are also very difficult to model and understand, as the micro- and macro-scales are intimately coupled, and making progress can require approaches that span the particle and continuum scales. I will discuss two examples motivated by recent experimental observations. In the first, I discuss numerical studies using classical nonlinear PDE models of viscoelastic flow at low Reynolds number. Using the extensional flow geometry of a four-roll mill, we have found symmetry breaking instabilities that give rise to multiple frequencies of flow oscillation, the appearance of coherent structures, and fluid mixing driven by small-scale vortex creation and destruction. In the second example, I will discuss recent modeling and simulations of active suspensions made up of many swimming particles. We find that such systems can stable or unstable at large-scales, depending upon the micro-mechanical swimming mechanism, and if unstable the flows have coherent structures whose stretch-fold dynamics yields rapid mixing.

**Anna-Karin Tornberg** (Stockholm) ***Model reduction for efficient simulation of fiber suspensions***

There is a strong anisotropy in the motion of slender rigid fibers. This anisotropy contributes to the very rich and complex dynamical behavior of fiber suspensions. The forming of "clusters" or "flocs" are purely three dimensional phenomena, and the direct simulation of these problems require simulations with many fibers for long times.

Earlier, we have developed a numerical algorithm to simulate the sedimentaion of fiber suspensions, considering a Stokes flow, for which boundary integral formulations are applicable. The algorithm is based on a non-local slender body approximation that yields a system of coupled integral equations, relating the forces exerted on the fibers to their velocities, which takes into account the hydrodynamic interactions of the fluid and the fibers. Even though there is a great gain in reducing a three-dimensional problem to a system of one-dimensional integral equations, the simulations are still computationally expensive, and the code has been parallelized and run on large computers to allow for more fibers and longer simulationtimes.

In this talk, I will present a model where approximations have been made to reduce the computational cost. Modifications have mainly been made concerning computation of long range interactions of fibers. The cost is substantially reduced by e.g. adaptively truncated force expansions and the use of multipole expansions combined with analytical quadrature.

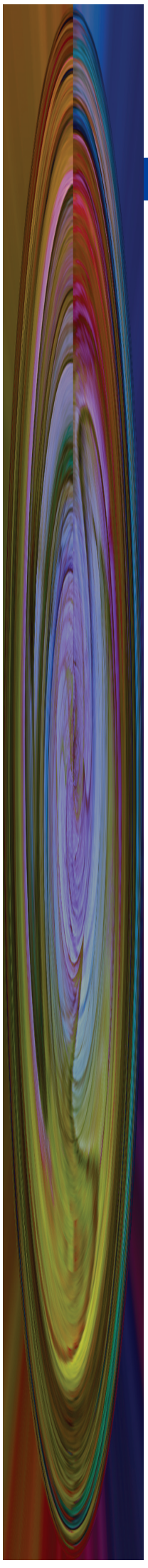
I will present results from various simulations and discuss the accuracy of the new model as I compare these results to results from large parallel simulations with the full model. A substantial reduction of the computational effort is normally attained, and the computational cost may comprise only a small fraction of the cost of the full model. This is however affected by parameters of the problem, such as the geometry and the fiber concentration, as will be discussed.

**Eric Vanden Eijnden** (Courant) ***Modeling and simulation of reactive events***

The dynamics of a wide range of systems involve reactive events, aka activated processes, such as conformation changes of macromolecules, nucleation events during first-order phase transitions, chemical reactions, bistable behavior of genetic switches, or regime changes in climate. The occurrence of these events is related to the presence of dynamical bottlenecks of energetic and/or entropic origin which effectively partition the phase-space of the dynamical system into metastable basins. The system spends most of its time fluctuating within these long-lived metastable states and only rarely makes transitions between them. The reactive events often determine the long-time evolution of the system one is primarily interested in. Unfortunately, computing up to the time scale at which these events occur represent an enormous challenge and so there is an urgent need for developing new numerical tools for such computations. One possibility is to build these numerical tools based on the Freidlin-Wentzell theory of large deviations which provides a complete picture of how and when rare events occurs in certain classes of systems. However, large deviation theory is valid in a parameter range where the random noise affecting the system is very small, which is often an inadequate assumption in complex systems. In addition, it becomes cumbersome to build numerical tools directly on Freidlin-Wentzell large deviation theory when the rare reactive events involves intermediates states, multiple pathways, etc. which is also the typical situation in high-dimensional systems. In this talk, I will explain why and describe a framework which allows to go beyond large deviation theory and can be used to identify the pathways and rate of rare reactive events in situations where the noise is not necessarily small, there are multiple pathways, etc. I will also describe numerical tools that can be built on this framework. Finally I will illustrate these tools on a selection of examples from molecular dynamics and material sciences.

**Darren Wilkinson** (Newcastle) ***Stochastic modelling and Bayesian inference for biochemical network dynamics***

This talk will provide an overview of computationally intensive methods for stochastic modelling and Bayesian inference for problems in computational systems biology. Particular emphasis will be placed on the problem of inferring the rate constants of mechanistic stochastic biochemical network models using high-resolution time course data, such as that obtained from single-cell fluorescence microscopy studies. The computational difficulties associated with "exact" methods make approximate techniques attractive. There are many possible approaches to approximation, including methods based on diffusion approximations, and methods exploiting stochastic model "emulators". Other important inferential problems will also be considered, such as inferring dynamic network connectivity from time course microarray data.



Tuesday 30 June – Friday 3 July 2009

# Capstone Conference

## Minisymposia Talks in the order in which they will be given

## Tuesday 30 June 2009 14:30–15:30 and 16:15–17:15

### Room MS.04 Organiser: **Jared Tanner**
*Sparse approximation and compressed sensing*

**Massimo Fornasier** (Massimo.Fornasier@oeaw.ac.at) *Inverse free-discontinuity problems and iterative thresholding algorithms*

Free-discontinuity problems describe situations where the solution of interest is defined by a function and a lower dimensional setconsisting of the discontinuities of the function. Hence, the derivative of the solution is assumed to be a "small function" almost everywhere except on sets where it concentrates as a singular measure. This is the case, for instance, in certain digital image segmentation problems.

1. In presence of an inverse problem, no existence results were available so far. First of all we show preliminary new results on the existence of minimizers for inverse free-discontinuity problems, by restricting the solutions to a class of functions which we called the Rondi's class.
2. If we discretize such situations for numerical purposes, the inverse free-discontinuity problem in the discrete setting can be re-formulated as that of finding a derivative vector with small components at all but a few entries that exceed a certain threshold. This problem is similar to those encountered in the field of "sparse recovery", where vectors with a small number of dominating components in absolute value are recovered from a few given linear measurements via the minimization of related energy functionals. As a second result, we show that the computation of global minimizers in the discrete setting is a NP-hard problem.
3. With the aim of formulating efficient computational approaches in such a complicated situation, we address iterative thresholding algorithms that intertwine gradient-type iterations with thresholding steps which were designed to recover sparse solutions. It is natural to wonder how such algorithms can be used towards solving discrete free-discontinuity problems. This talk explores also this connection, and, by establishing an iterative thresholding algorithm for discrete inverse free-discontinuity problems, provides new insights on properties of minimizing solutions thereof.

This is partially a joint work with Riccardo March (CNR, Italy) and Rachel Ward (PACM, Princeton University, USA).

**Mike Davies** (Mike.Davies@ed.ac.uk) *Sparse signal recovery: alternatives to L1*

Finding sparse solutions to underdetermined inverse problems is a fundamental challenge encountered in a wide range of signal processing applications, from signal acquisition to source separation. Recent theoretical advances in our understanding of this problem have further increased interest in their application to various domains. In many areas, such as for example medical imaging or geophysical data acquisition, it is necessary to find sparse solutions to very large underdetermined inverse problems. Fast methods therefore have to be developed. In this talk, we will present fast algorithms that are competitive with the more classical convex L1 minimization (Basis Pursuit) technique. These methods will instead work more directly on the non-convex L0 optimisation function. One such strategy is the extremely simple algorithm called Iterative Hard thresholding (IHT). Despite its simplicity it can be shown that: it gives near-optimal performance guarantees; it is robust to observation noise; it has low bounded computational complexity per iteration and only requires a fixed number of iterations depending on the signal to noise ratio of the signal. Unfortunately a niaive application of IHT yields empirical performance substantially below that of other state of the art recovery algorithms. We therefore discuss have the algorithm can be modified to obtain performance that is comparable with state of the art while retaining its strong theoretical properties.

**Rémi Gribonval** (Remi.Gribonval@inria.fr) H*ow many training samples does it take to learn a dictionary for sparse representations?*

We consider the problem of learning a dictionary providing sparse representations for a given signal class, via $\ell_1$-minimisation. The problem can also be seen as factorising a $d \times N$ matrix $Y=(y_1 \ldots y_N), \, y_n\in \mathbb{R}^d$ of training signals into a $d \times K$ dictionary matrix $\mathbf{\Phi}$ and a $K \times N$ coefficient matrix $X=(x_1\ldots x_N),\, x_n \in \mathbb{R}^N$, which is sparse. The exact question studied here is when a dictionary coefficient pair $(\mathbf{\Phi},X)$ can be recovered as local minimum of a (nonconvex) $\ell_1$-criterion with input $Y=\mathbf{\Phi} X$. First, for general dictionaries and coefficient matrices, algebraic conditions ensuring local identifiability are derived, which are then specialised to the case when the dictionary is a basis. Finally, assuming a random Bernoulli-Gaussian sparse model on the coefficient matrix, it is shown that sufficiently incoherent bases are locally identifiable with high probability. The perhaps surprising result is that the typically sufficient number of training samples $N$ grows (up to a logarithmic factor) only linearly with the signal dimension, i.e. $N \approx C K \log K$, in contrast to previous approaches requiring combinatorially many samples.

**Jared Tanner** (jared.tanner@ed.ac.uk) *Phase transitions phenomenon in compressed sensing*

Compressed Sensing has broken the Nyquist barrier, but what is the sampling theorems for CS? Reconstruction algorithms typically exhibit a phase transition phenomenon for large problem sizes, where there is a domain of problem sizes for which successful recovery occurs with overwhelming probability, and there is a domain of problem sizes for which recovery failure occurs with overwhelming probability. These phase transitions serve as sampling theorems for CS. The mathematics underlying this phenomenon will be outlined for L1 regularization and non-negative feasibility point regions. Both instances employ a large deviation analysis of the associated geometric probability event. These results give precise if and only if conditions on the number of samples needed in Compressed Sensing applications. Lower bounds on the phase transitions implied by the Restricted Isometry Property for Gaussian random matrices will also be presented for the following algorithms: Lq-regularization for q between zero and one, CoSaMP, Subspace Pursuit, and Iterated Hard Thresholding. This work is joint with Blanchard, Cartis, Donoho, and Thompson.

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### Room MS.05 Organiser: **Omiros Papaspiliopoulos** *Stochastic modelling and computer-intensive inference in biology*

**Simon Cauchemez** (Imperial) *Early spread of the novel Influenza A(H1N1) virus: insights from mathematical modelling*

I will discuss the work of the MRC Centre for Outbreak Analysis and Modelling at Imperial College on the unfolding novel Influenza A(H1N1) pandemic. Staff of the MRC Centre have been working with US CDC, the UK Health Protection Agency, the World Health Organisation and the Mexican government to understand the early spread of this new influenza virus. Early work has focussed on understanding the transmission dynamics of the virus and estimating key epidemiological parameters. I will discuss

the challenges of real-time outbreak analysis, such as working with ever-changing and incomplete data, and needing to draw preliminary conclusions when underlying uncertainty is huge.

**Mark Girolami** (Glasgow) *Efficiently performing bayesian inference over dynamical biochemical system models with hamiltonian monte carlo on the riemann manifold*

Formally characterising uncertainty in systems of differential equations within a statistical inferential framework is something which mathematicians and statisticians have only very recently started to consider. There is great motivation within the area of Computational Systems Biology to fully define and propagate all sources of uncertainty in model-based reasoning regarding the biochemical mechanisms initiating and regulating fundamental biological processes. The Bayesian methodology provides such an inferential framework, however, whilst beautifully elegant in principle the computational statistical challenges associated with its practical instantiation are formidable. This talk presents two contributions in addressing such challenges, the first presents a statistically and computationally efficient Markov Chain Monte Carlo Sampler for systems of nonlinear differential equations by the introduction of auxiliary functional processes into the overall model. The second contribution defines a non-separable Hamiltonian defined on the Riemann manifold and an explicit time reversible symplectic integrator is developed which provides a means of performing Hybrid Monte Carlo on the manifold defined by the nonlinear dynamic system described by the system of equations. Convergence to the stationary distribution in cases of, for example, time-delayed differential equations is improved four-hundred fold, additional biochemical model examples related to Circadian control in plants will be presented.

**Michael Stumpf** (Imperial) *An approximate Bayesian computation perspectives on learning the structure of biological signalling systems from time-course data.* Joint work with Kamil Erguler, Paul Kirk, Juliane Liepe, Maria Secrier and Tina Toni

For the vast majority of biological systems we lack reliable models let alone model parameters. Using well defined simulation models and real biological data collected for a range of biological signalling systems, we explore how much can be learned about biological systems from temporally resolved transcriptomic or proteomic data. We pay particular attention to qualitative properties of the underlying dynamical system and their impact on our ability to infer the system's dynamics. We then illustrate how approximate Bayesian computation approaches can be employed to gain insights into the inferability of model parameters, and for model selection in the context of dynamical systems in biology.

**Barbel Finkelstadt** (Warwick) *Inferring molecular degradation rates in single cells: An application of Bayesian hierarchical modeling to SDEs.* Joint with Dan J. Woodcock, Michal Komorowski, David A. Rand. Experiments: Claire V. Harper, Julian R. E. Davies, Michael R. H. White

Understanding biological processes at the molecular level is an important aspect of studying cellular phenomena. Recent development in fluorescent microscopy technology enabled us to measure levels of reporter proteins in vivo such as green fluorescent protein (GFP) and luciferase (luc) in individual cells. The understanding of how the observed fluorescence level relates to the dynamics of gene expression is facilitated by the knowledge of mRNA and reporter protein degradation rates. Provided with replicate single cell protein data we present a modeling approach together with a statistical methodology that overcomes many of the current problems in the estimation of the degradation rates. We formulate a suitable SDE model that has both the protein and the mRNA degradation rates as parameters. These can be inferred sequentially from the reporter protein data from two types of experiments where either transcription or translation is inhibited. The corresponding inference algorithm is challenging as we are confronted with a two-dimensional SDE system where one of the variables (mRNA abundance) is unobserved and the second variable (protein abundance) is measured discretely in time with measurement error. In order to quantify the extrinsic noise due to variation of the degradation between cells this model is extended towards a Bayesian hierarchical model.

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## Room B3.02 Organiser: Steve Coombes
### *Mathematical neuroscience*

**Peter Ashwin** (Exeter) *Winnerless competition for coupled neural dynamics*

Idealized models of neural dynamics (such as neural networks) tend to make much use of variational dynamics, by assuming the presence of an "energy functional". These models suggest that neural computations occur by following a path that successively minimizes this functional, but there is no particular reason to believe that such a functional exists except possibly locally in phase space. Work in the past few years by Huerta, Rabinovich and others has suggested that certain neural processes work instead by means of "winnerless competition". In such models this translates into dynamics that explores many dimensions but in a very structured way: a heteroclinic attractor. This talk with discuss some recent work on neurally plausible models that give rise to such dynamics, and how this could be of relevance to cognitive puzzles such as binocular rivalry and neural resting states.

**Antoni Guillamon** (Barcelona) *Phase resetting surfaces: extending phase resetting curves out of the periodic attractors*

The knowledge of the phase advancement after a given stimulus is an important point for the control of biological oscillators. We will present a numerical method to perform the effective computation of the phase advancement when we stimulate an oscillator which has not reached yet the asymptotic state (a limit cycle). That is, we extend the computation of the phase resetting curves (the classical tool to compute the phase advancement) to a neighborhood of the limit cycle, obtaining what we call the phase resetting surfaces (PRS). To achieve this goal we first perform a careful study of the theoretical grounds (the parameterization method for invariant manifolds and another approach using Lie symmetries), which allows to describe the isochronous sections of the limit cycle and, from them, to obtain the PRSs. We will explain how we make this theoretical framework applicable, by using the numerical algorithms of the parameterization method and other semianalytical tools to extend invariant manifolds; as a result, we design a numerical scheme to compute both the isochrons and the PRSs of a given oscillator. Finally, to illustrate this algorithm, we will show its application to some well-known biological models. We will put strong emphasis in the biological implications and provide new examples that reinforce the usefulness of the phase resetting surfaces.

**Carlo Laing** (Massey) *Dimension reduction in neural models: an example – binocular rivalry*

Binocular rivalry occurs when two very different images are presented to the two eyes. Previous models for this phenomenon have been either phenomenological rate models or more realistic spiking neuron models. Few attempts have been made to derive the former type of model from the latter. We give such a derivation, using data-mining techniques to automatically extract appropriate variables for a low-dimensional description.

**Yulia Timofeeva** (Warwick) *Mathematics of dendritic democracy*

Neurons receive synaptic inputs primarily onto their dendrites, which filter synaptic potentials as they spread toward the soma. There is experimental evidence that synaptic efficacy increases as a function of distance from the soma. Distance dependent synaptic scaling is just one of several mechanisms for achieving so-called "dendritic democracy" whereby the spatially extended single neuron can compensate for dendritic attenuation. In my talk I will demonstrate how this phenomenon can be explored from a mathematical perspective for both idealised and realistic dendritic geometries.

# Wednesday 1 July 2009 14:30–15:30 and 16:15–17:15

## Room MS.04 Organiser: Nancy Nichols
*Model reduction*

**Carsten Hartmann** (Frei, Berlin) *Balanced model reduction of hamiltonian systems*

We study model reduction of partially-observed linear Hamiltonian systems that are subject to an external perturbation. Large-scale systems of this kind arise in a variety of physical contexts, e.g., in molecular dynamics or structural mechanics. Common spatial decomposition methods such as the Principal Component Analysis aim at identifying a subspace of "high-energy" modes onto which the dynamics are projected. These modes, however, may not be relevant for the dynamics. Moreover the methods tacitly assume that all degrees of freedom can actually be observed or measured. Balanced model reduction consists in (1) transforming the system such that those degrees of freedom that are least sensitive to the perturbation also give the least output and (2) neglecting the respective unobservable/uncontrollable modes. The second step is not unique, and, from the perspective of structure-preservation, it matters how the negligible modes are eliminated; for example, projecting the dynamics onto the essential subspace destroys the underlying Hamiltonian structure. We explain how balanced model reduction can be carried out in a structure-preserving fashion, including preservation of stability and passivity.

**Nancy K. Nichols** (Reading) *Model reduction by balanced truncation for unstable, α-bounded systems*

(Jt authors: C. Boess, A. Bunse-Gerstner, A.S. Lawless)

Model reduction techniques based on balanced-truncation require that the system model is stable; otherwise, the methods are able to reduce only the stable part of the system. For systems that have very large unstable parts, which often arise in the geosciences and in environmental applications, significant reductions in the model size are therefore not possible. Here we describe a new method for model reduction for unstable linear systems that are 'α-bounded', that is, systems for which the eigenvalues of the system matrix lie in a disc of radius α around the origin. The new method uses balanced truncation to determine a reduced order model that satisfies the first order necessary conditions for an optimal approximation in the h2,α-norm. A bound on the error between the transfer functions of the original system and the reduced order system obtained by this method is given in the h∞,α-norm. In numerical experiments, the significant unstable and stable modes of the system are captured effectively by the reduced models and the results demonstrate a superior performance using the α-bounded reduction technique in comparison to the standard balanced truncation method for systems with many unstable modes.

**Angelika Bunse-Gerstner** (Bremen) *Interpolation-based model reduction for data assimilation*

(Jt authors: C. Boess, N.K. Nichols, D. Kubalinska

Model reduction methods have already shown a potential to improve the computational efficiency of data assimilation schemes. They decrease the computational complexity considerably by generating reduced order linear dynamical systems which behave similarly to the linearisations of the model for the environmental systems used within the Gauss-Newton iteration steps. To make this approach feasible for realistic problems we need model reduction methods that can handle the very large dimensions of the original systems. Numerical methods based on rational tangential interpolation are attractive for these very large dimensions. Moreover, it can be shown that interpolation data can be chosen such that the reduced order dynamical system satisfies first order necessary conditions for an optimal approximation in the h2,α-norm. In this talk we discuss various properties as well as the computation of such reduced order models for very large systems and show experimental results. In particular it is shown how this method is related to an approximate computation of the extremely useful but computationally very expensive balanced truncation model reduction.

**Arnold Heemink** (Delft) *Model reduced variational assimilation* (Jt authors: M.U. Altaf, M.P Kaleta)

Data assimilation methods are used to combine the results of a large scale numerical model with the measurement information available in order to obtain an optimal reconstruction of the dynamic behavior of the model state. Variational data assimilation or "the adjoint method" has been used very often for data assimilation. This approach is especially attractive for model calibration problems. Using the available data, the uncertain parameters in the model are identified by minimizing a certain cost function that measures the difference between the model results and the data. In order to obtain a computational efficient procedure, the minimization is performed with a gradient-based algorithm where the gradient is determined by solving the adjoint problem.

Variational data assimilation requires the implementation of the adjoint model. Even with the use of the adjoint compilers that have become available recently this is a tremendous programming effort, that hampers new applications of the method. Therefore we propose another approach to variational data assimilation using model reduction that does not require the implementation of the adjoint of (the tangent linear approximation of) the original model. Model reduced variational data assimilation is based upon a POD (Proper Orthogonal Decomposition) approach to determine a reduced model for the tangent linear approximation of the original nonlinear forward model. Once this reduced model is available, its adjoint can be implemented very easily and the minimization process can be solved completely in reduced space with negligible computational costs. If necessary, the procedure can be repeated a few times by generating new ensembles more close to the most recent estimate of the parameters.

In the presentation we will introduce the model reduced variational data assimilation approach. The characteristics and performance of the method will be illustrated with a number of real life data assimilation applications to oil reservoir models and coastal sea models.

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## Room MS.05 Organiser: Colin Cotter
*Lagrangian structure, Lagrangian data*

**Simon Cotter** (Warwick) *Lagrangian data assimilation for a viscous incompressible fluid*

(Collaboration with Masoumeh Dashti, James Robinson and Andrew Stuart)

We study the inverse problem of determining the initial state, and possibly the forcing, of a viscous incompressible fluid observed indirectly through the positional data from passive Lagrangian tracers, over a period of time. We formulate this as a Bayesian inverse problem, giving rise to a probability measure on function space for the initial vector field, and the forcing (or model error). We will describe a well-posed mathematical setting for this problem and describe the results of effective MCMC methods that allow us to sample from such a posterior distribution.

**Shane Elipot** (Proudman Oceanographic Laboratory) *The transfer function for wind-driven oceanic currents*

The international oceanographic community maintains an "array" of approximately 1200 freely-drifting buoys at the surface of the World Ocean. These Lagrangian surface "drifters" are drogued at 15 m depth so that their displacements with time are representative of near-surface currents. A large component of the variance of these currents is ascribable to direct forcing by the atmospheric wind stress.

The drifter velocity data, combined with wind data, are used to infer the transfer function in the spectral domain from the

atmospheric wind stress to the wind-driven current. In order to interpret physically the observed response to atmospheric forcing, these observations are compared to theoretical transfer functions arising from a suite of theoretical models for the oceanic top boundary layer.
Some general mathematical properties of these transfer functions are discussed and it is shown in particular that the boundary conditions of the theoretical models are crucial in setting their limiting behavior around the resonant inertial frequency.

**Emilio Hernandez-Garcia** (IFISC CSIC-UIB) *Stretching fields and lines in ocean transport dynamics*
Developments of the Lagrangian description of fluid motion have allowed the introduction of dynamical systems tools into the characterization of transport dynamics and mixing in fluid flows. In this talk I will describe applications, mainly based in the use of the finite-size Lyapunov exponent, of these ideas to understanding transport in ocean flows. The techniques are flexible enough to deal with velocity fields obtained by simulation and by satellite altimetry observations. Plankton and marine birds are shown to be affected by the physical ocean structures revealed by the Lyapunov analysis.

**Jonathan Lilly** (Earth and Space Research) *Inferring oceanic vortex properties from Lagrangian data* Joint work with Sofia Olhede, UCL
The large amounts of data from freely – drifting, or "Lagrangian", subsurface floats have opened a unique window into the structure and variability of the deep ocean currents. Plots of the trajectories from these floats are typically called "spaghetti diagrams" because of their chaotic and frequently looping character. We have developed a method to use this data to infer the properties of oceanic vortices, also known as "coherent eddies". Such vortices are known to be important for transport and mixing of heat and salt, but are difficult to parameterize in models on account of their longevity and ability to translate long distances.
Our method is based on an extension of the ideas of "instantaneous moments" for the analysis of non-stationary (i.e., inhomogeneous in time) univariate signals to the bivariate case. Estimation of the time-varying instantaneous moments is accomplished via a generalization of wavelet ridge analysis to multivariate signals. Random fluctuations – due to instrument noise and the red background flow–lead to stochastic distributions of the estimated instantaneous moments, which we solve for.
Due to a direct relationship between eddy properties and the instantaneous moments of a bivariate oscillation, important aspects of the eddy structure such as its time-varying vorticity can then be inferred, and bounded by error bars. This formalizes an automated and objective solution for the extraction of vortex structures, a task which has hitherto been accomplished by more subjective means.

## Room B3.02 Organiser: **Ben Leimkuhler**
### *Molecular dynamics in and out of equilibrium*

**Ruslan Davidchack** (Leicester) *Discretisation errors in MD simulations with deterministic and stochastic thermostats*
We investigate the influence of numerical discretisation errors on computed averages in molecular dynamics simulations with deterministic and stochastic thermostats, and discuss possible approaches to estimating such errors and taking them into account when computing the averages. In most cases this enables the use of larger integration time steps than those typically considered acceptable by the MD practitioners.

**Frédéric Legoll** (ENPC, Paris) *Parareal algorithms and long-time integration of Hamiltonian systems*
Time integration schemes for ODEs are naturally sequential in time. The parareal algorithm, proposed in 2001, was one of the first efficient integration schemes that include some parallel computations. Since then, it has been successfully used on many different equations.
Our aim is to get a better understanding of the long-time properties of such an approach, that are of paramount importance when the scheme is used to integrate Hamiltonian systems. We will present several modifications of the original scheme, aiming at improving its long-time behaviour.

**Nawaf Bou-Rabee** (New York) *Metropolized integrators for SDEs*
Metropolis adjusted integrators for stochastic differential equations (SDE) are presented which (i) are ergodic with respect to the exact equilibrium distribution of the SDE and (ii) approximate pathwise the solutions of the SDE on finite time intervals. Both these properties are demonstrated and precise strong error estimates are derived. It is also shown that the Metropolized integrator retains these properties even in situations where the drift in the SDE is nonglobally Lipschitz, and vanilla explicit integrators for SDEs typically become unstable and fail to be ergodic. This talk is based on a joint paper with Eric Vanden-Eijnden.

**Emad Noorizadeh** (Edinburgh) *The concept of heat bath in molecular dynamics*
A heat bath in molecular dynamics is a perturbation of the Hamiltonian dynamics which enables correct computation of ensemble averages. On the other hand computation of dynamical averages such as autocorrelation functions requires the molecular dynamics trajectory to be close to a microcanonical dynamics. This suggests that, ideally, we would like to have a small growth of the perturbation together with a fast rate of convergence to the Boltzmann-Gibbs measure. In this talk we try to quantify the rate of convergence to equilibrium and the growth of the perturbation for Langevin dynamics and the Hoover-Langevin method (a highly degenerate diffusion). We illustrate our results using numerical experiments. This is joint work with Ben Leimkuhler and Oliver Penrose.

# Thursday 2 July 2009 14:30–15:30 and 16:15–17:15

## Room MS.04 Organiser: Mike Allen
*Future directions in molecular simulation*

**Marjolein Dijkstra** (Utrecht) *Do smectic nuclei exist?*

The smectic phase is a well-known liquid crystalline state of matter in which elongated particles form parallel stacks of fluid-like layers. However, the formation of a smectic phase and the nature of the transient structures (clusters, nuclei, droplets) are still a mystery. Whereas the existence of gas-bubbles in a superheated liquid, liquid droplets in a supersaturated gas, or crystallites in an undercooled liquid are undisputed transient structures, there seems to be no analogue for smectic clusters: simple transient smectic droplets have never been observed to the best of our knowledge. Using computer simulations, we have studied the formation of the smectic phase in suspensions of colloidal hard rods and in mixtures of rods and non-adsorbing polymer. We find that the nucleation of the smectic phase is hampered for pure rods due to slow dynamics as the density of the isotropic fluid phase is very high. When polymer coils are added to the suspension, an effective attraction between the rods is induced and we observe nucleation and growth at relatively high supersaturation. More suprisingly, perhaps, we observe that the critical nucleus consists of a single layer of rods and that multiple layers of the smectic phase are formed only due to coalescence of single layers of rods.
In addition, we study the stability of orientationally disordered crystal phases in a suspension of colloidal hard dumbbells using Monte Carlo simulations. We find that the plastic crystal with the hcp structure is more stable than the fcc structure, while it is well-known that for hard spheres the fcc structure is more stable. In addition, we find that the orientationally disordered aperiodic crystal structure is a stable phase in the phase diagram. Moreover, we determine the phase behaviour of colloidal shells (bowls) and we find a remarkably rich variety of liquid crystalline phases as a function of the thickness of the shells. We compare our results with experiments on colloidal dumbbells and colloidal shells.

**Alessandro Troisi** (Warwick) *An unexpected application of classical molecular simulations: understanding the quantum dynamics of the electrons in soft materials* Co-Authors: D. Cheung, D. McMahon (University of Warwick), D. Andrienko (MPIP - Mainz)

The charge dynamics in many soft materials (semiconducting polymers and liquid crystals) is controlled by the nuclear dynamics and an efficient evaluation of the latter is now recognized as one of the most difficult tasks toward the prediction of the electronic properties of these materials. We present two recent examples of our method to predict the charge mobility based on a combination of classical and quantum simulations: (i) the P3HT polymers in the crystalline phase and the electronic traps induced by his conformational dynamics, (ii) the charge dynamics in a columnar liquid crystal where a model based on Langevin dynamics can be used to extract the charge mobility.

**Richard Vink** (Göttingen) *Monte Carlo simulations of fluids with quenched disorder*

It is well known that the liquid-gas transition in a fluid belongs to the universality class of the Ising ferromagnet. This means that critical exponents measured in a fluid are identical to those of the Ising model, even though the systems are obviously very different. In this presentation, I will discuss the more complicated problem of a fluid mixture consisting of mobile particles and immobile ones. As it turns out, the universality class of such a system is that of the random-field Ising model.

**Nigel Wilding** (Bath) *Simulations studies of polydisperse crystals*

Many complex fluids are polydisperse, that is they comprise mixtures of similar rather than identical constituents. Examples are colloidal dispersions in which the particles may exhibit a spread of sizes, shapes or surface charges, or polymers which may have a range of chain lengths. In this talk I will outline some of the interesting effects polydispersity can have on bulk phase behaviour. I will then describe the computational challenges posed by polydispersity and describe new Monte Carlo simulation algorithms that allow the phase behaviour of polydisperse systems to be tackled effectively. Simulations results for the influence of size polydispersity on the crystalline phase of soft spheres will then be presented. Polydispersity is seen to give rise to pronounced changes in the melting properties and to the appearance of multiple coexisting fcc solid phases at high *densities*.

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## Room MS.05 Organiser: Coralia Cartis
*Optimization*

**Pierre-Antoine Absil** (Louvain) *Accelerated optimization methods and their convergence*

Let $T$ be a descent mapping for a differentiable real-valued function $f$. Let $(x_k)$ be a "$T$-accelerated" sequence, namely, there is $c>0$ such that, for all $k$, $f(x_k) - f(x_{k+1}) \geq c (f(x_k) - f(T(x_k)))$. We propose weak conditions on $T$ that ensure that every accumulation point of $(x_k)$ is a critical point of $f$. This theory has applications, e.g., in the analysis of eigenvalue algorithms and of certain types of switched discrete-time systems.

**Frank E. Curtis** (Courant) *Inexact Newton methods for nonlinear constrained optimization*

Inexact Newton methods play a fundamental role in the solution of large-scale unconstrained optimization problems and nonlinear equations. The key advantage of these approaches is that they can be made to emulate the properties of Newton's method while allowing flexibility in the computational cost per iteration. Due to the multi-objective nature of *constrained* optimization problems, however, that require an algorithm to find both a feasible and optimal point, it has not been known how to successfully apply an inexact Newton method within a globally convergent framework. In this talk, we present a new methodology for applying inexactness to the most fundamental iteration in constrained optimization: a line-search primal-dual Newton algorithm. We illustrate that the choice of merit function is crucial for ensuring global convergence and discuss novel techniques for handling non-convexity, ill-conditioning, and the presence of inequality constraints in such an environment. Preliminary numerical results are presented for PDE-constrained optimization problems.

**Raphael Hauser** (Oxford) *Adversarial smoothed analysis*
Coauthors: Martin Lotz, Felipe Cucker.

We present smoothed analysis bounds for conic condition numbers under a general class of radially symmetric perturbation distributions around an input data point of a numerical problem. The generality of our theory is such that it applies to the conditioning of a family of important problems in numerical analysis and to perturbation distributions whose density can have a singularity at the center of the perturbation, a class of distributions we call **adversarial**.

**Michal Kocvara** (Birmingham) *On the solution of large-scale semidefinite problems in structural optimization*

We propose a new approach for solving the structural optimization problems where stability of the optimal structure is enforced either by vibration control, that is control of the fundamental eigenfrequency, or by control of the critical buckling load. The problem leads to a large-scale nonlinear programming problem. When stability control in enforced, a large and sparse semidefinite constraint

is added to this problem; in the case of the critical buckling load, this constraint is nonlinear. Such problems are demanding from the viewpoint of computational cost, due to the dimension of real life instances. In particular, the problems are characterized by a large number of variables and, at the same time, a high dimension of the matrix constraint. This kind of problems is impossible to solve by recent semidefinite programming software based on interior point methods. Our approach is based on a nonlinear reformulation of the positive semidefinite constraint which was first proposed by Fletcher. It applies to linear as well as nonlinear semidefinite constraints. The resulting nonlinear program is solved by a variant of the Method of Moving Asymptotes, which is popular and provably efficient in Structural Optimisation. A working set strategy is also introduced in order to save computational effort. This is a joint Work with Claudio Bogani (University of Birmingham) and Michael Stingl (University of Erlangen).

## Room B3.02 Organiser: Endre Suli

*Numerical analysis of nonlinear evolution equations*

**John W. W. Barrett** (Imperial College) *Parametric approximation of geometric evolution equations*
Co-authors Harald Garcke, Robert Nürnberg.

Geometric flows, in which hypersurfaces move such that an energy, involving surface and bending terms, decreases appear in many situations in the natural sciences and in geometry. Classic examples are mean curvature, surface diffusion and Willmore flows. Computational methods to approximate such flows are based on one of three approaches (i) parametric methods, (ii) phase field methods or (iii) level set methods. The first tracks the hypersurface, whilst the other two implicitly capture the hypersurface. A key problem with the first approach, apart from the fact that it is does not naturally deal with changes of topology, is that in most cases the mesh has to be redistributed after every few time steps to avoid coalescence of mesh points.
In this talk we present a variational formulation of the parametric approach, which leads to an unconditionally stable, fully discrete finite element approximation. In addition, the scheme has very good properties with respect to the distribution of mesh points, and if applicable volume conservation. We illustrate this for (anisotropic) mean curvature and (anisotropic) surface diffusion flows of closed curves in $\mathbb{R}^2$ and closed hypersurfaces in $\mathbb{R}^3$. We extend these flows to curve networks in $\mathbb{R}^2$, and surface clusters in $\mathbb{R}^3$. Here the triple junction conditions, that have to hold where three curves/surfaces meet at a point/line, are naturally approximated in the discretization of our variational formulation. Finally, we extend these approximations to the case when the hypersurface motion depends also on an under-lying background equation, such as the Stefan problem with kinetic undercooling and the Mullins–Sekerka/Hele–Shaw flow with surface tension.

**Sören Bartels** (Bonn) *Robust approximation of phase field models past topological changes*

Phase field models are often used to describe the evolution ofsubmanifolds, e.g., the Allen-Cahn equation approximates motion by meancurvature and more sophisticated phase field models provideregularizations of Willmore flow and other geometric evolution problems.The models involve small regularization parameters and we discuss thedependence of a priori and a posteriori error estimates for thenumerical solution of the regularized problems on this parameter. Inparticular, we address the question whether robust error estimation ispossible past topological changes. We provide an affirmative answer fora priori error estimates assuming a logarithmic scaling law of the timeaveraged principal eigenvalue of the linearized Allen-Cahn or Ginzburg-Landau operator. This scaling law is confirmed by numericalexperiments for generic topological changes. The averaged eigenvalueenters a posteriori error estimates exponentially and therefore,critical scenarios are detected automatically by related adaptive finiteelement methods.

**Charlie Elliott** (Warwick) *Computational evolutionary PDEs on surfaces*

Evolutionary PDEs on stationary and moving surfaces appear in many applications such as the diffusion of surfactants on fluid interfaces, surface pattern formation on growing domains, segmentation on curved surfaces and phase separation on biomembranes and dissolving alloy surfaces. In this talk I discuss recent work with G. Dziuk (Freiburg) on novel finite element methods on triangulated surfaces and implicit surfaces defined as level sets.

**Endre Suli** (Oxford) *Analysis and approximation of coupled Navier-Stokes-Fokker-Planck systems in kinetic models of dilute polymers* (Co-authors John W. Barrett, David J. Knezevic)

We review recent analytical and computational results for macroscopic-microscopic bead-spring models that arise from the kinetic theory of dilute solutions of incompressible polymeric fluids with noninteracting polymer chains, involving the coupling of the unsteady Navier–Stokes system in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3, with an elastic extra-stress tensor as right-hand side in the momentum equation, and a (possibly degenerate) Fokker–Planck equation over the $(2d + 1)$-dimensional region $\Omega \times D \times [0,T]$, where $D \subset \mathbb{R}^d$ is the configuration domain and $[0, T]$ is the temporal domain. The Fokker–Planck equation arises from a system of (Itô) stochastic differential equations, which models the evolution of a $2d$-component vectorial stochastic process comprised by the $d$-component centre-of-mass vector and the d-component orientation (or configuration) vector of the polymer chain. We show the existence of global-in-time weak solutions to the coupled Navier–Stokes–Fokker–Planck system for a general class of spring potentials including, in particular, the widely used finitely extensible nonlinear elastic (FENE) potential. The numerical approximation of this high-dimensional coupled system is a formidable computational challenge, complicated by the fact that for practically relevant spring potentials, such as the FENE potential, the drift term in the Fokker–Planck equation is unbounded on $\partial D$.

# Friday 3 July 2009 10:00–11:00 and 11:45-12:45

## Room MS.04 Organiser: Greg Pavliotis
*Numerical methods for multiscale stochastic systems*

**C. Hartmann** (FU Berlin) *Model reduction of partially-observed Langevin equations*
We study balanced model reduction of a certain class of stochastic dif ferential equations. In doing so, we adopt ideas from large deviations theory and discuss notions of controllability and obervability for linear dissipative Hamiltonian systems with degenerate noise term, also known as Langevin equations. For partially observed Langevin equations, we illustrate model reduction by balanced truncation with an example from molecular dynamics and discuss aspects of structure-preservation.

**M. Katsoulakis** (U. Crete and U. Mass Amherst) *Hierarchical and multi-level coarse-graining methods*
We will discuss a variety of coarse-graining methods for many-body microscopic systems. We focus on mathematical, numerical and statistical methods allowing us to assess the parameter regimes where such approximations are valid. We also demonstrate, with direct comparisons between microscopic (DNS) and coarse-grained simulations, that the derived mesoscopic models can provide a substantial CPU reduction in the computational effort.
Furthermore, we discuss the feasibility of spatiotemporal adaptivity methods for the coarse-graining of microscopic simulations, having the capacity of automatically adjusting during the simulation if substantial deviations are detected in a suitable error indicator. Here we will show that in some cases the adaptivity criterion can be based on a posteriori estimates on the loss of information in the transition from a microscopic to a coarse-grained system.
Finally, motivated by related problems in the simulation of macromolecular systems, we discuss mathematical strategies for reversing the coarse-graining procedure. The principal purpose of such a task is recovering local microscopic information in a large system by first employing inexpensive coarse-grained solvers.

**F. Legoll** (ENPC) *Effective dynamics using conditional expectations*
We consider a system described by its position $X_t$ , that evolves according to the overdamped Langevin equation, and a scalar function $\xi(X)$ of the state variable $X$. Our aim is to design a one-dimensional dynamics that approximates the evolution of $\xi(X_t)$. Using conditional expectations, we build an original dynamics, whose accuracy is supported by error estimates between the laws of the two processes, at any fixed time. Simple numerical simulations illustrate the efficiency of the approach as well as the accuracy of the proposed dynamics according to various criteria, including residence times in potential energy wells.

**K.C. Zygalakis** (Oxford) *On the existence and applications of modified equations for stochastic differential equations*
In this talk we describe a general framework for deriving modified equations for stochastic differential equations with respect to weak convergence. Results are presented for first order methods such as the Euler-Maruyama and the Milstein method. In the case of linear SDEs, using the Gaussianity of the underlying solutions, we derive a SDE which the numerical method solves exactly in the weak sense. Applications of modified equations in the numerical study of Langevin equations and in the calculation of effective diffusivities are also discussed.

## Room MS.05 Organiser: Jason Frank
Computational methods for geophysical flows

**Matthias Lauter** (Alfred Wegener Institute) *A semi-implicit discontinuous Galerkin Method for non-hydrostatic and hydrostatic atmospheric flows*
The vertical structure of the averaged free atmosphere is dominated by the hydrostatic balance. The propagation of waves with horizontal spatial scales larger than 10km is similar in a model based on non-hydrostatic and hydrostatic flow equations. Wave speeds and the dispersion properties of shorter wave lengths differ significantly in for both equation sets.
A non-hydrostatic as well as a hydrostatic equation set is considered in a 2d mesoscale atmospheric model setup. We apply a high order discontinuous Galerkin method with a semi-implicit time stepping on a terrain following quadrilateral grid. Dispersion relations, wave propagation and experimental convergence studies are performed to validate the proposed method with respect to established atmospheric test cases.
Authors: Matthias Laeuter (Alfred Wegener Institute, Germany), Francis X. Giraldo (Naval Postgraduate School, USA), Marco Restelli (Max Plank Institut for Meteorology, Germany), Sebastian Reich (University Potsdam, Germany), Darthe Handorf (Alfred Wegener Institute, Germany), Klaus Dethloff (Alfred Wegener Institute, Germany).

**Hilary Weller** (Reading) *Adaptive Mesh Modelling of the Global Atmosphere*
Adaptive meshing of the atmosphere may prove beneficial for resolving tropical cyclones, fronts, convection and orography. However there are a number of challenges before these methods can be effective operationally. These include finding appropriate mesh refinement criteria, automatic re-meshing for unstructured meshes and conservative mesh to mesh mapping which does not alter the partition between balanced and unbalanced fields. I will describe a new model of the global atmosphere which solves the shallow water equations accurately on any mesh of the sphere. This has allowed direct comparisons between different mesh structures and different refinement patterns. I will also describe a new mesh refinement technique which allows infrequent mesh adaptation. This reduces the cost of remeshing and reduces the errors introduced by remeshing.

**Matthias Sommer** (Berlin) *A conservative scheme for the shallow-water system and its statistical and geometrical properties*
As is well known, the geometrical description of a dynamical system by means of the (generalised) Hamiltonian representation can be useful for the understanding of its conservative, geometric and statistical properties. In numerics, this method has recently been applied to spatial and temporal discretisations of fluid dynamical systems. Here, it will be shown how such a generalised Hamiltonian/Nambu approach can be used to construct a conservative spatial semi-discretisation of the shallow-water equations on a staggered geodesic grid. Numerical experiments will demonstrate this scheme's capability of representing essential conservation properties of the full (PDE) system and how this affects stability and spectral behaviour. Phase space geometrical and statistical properties of the scheme will also be discussed.

**Onno Bokhove** (Twente) *Hamiltonian water wave model -with accurate dispersion and vertical vorticity*
1. Luke's variational principle for potential flow waves has been extended to flows with vertical vorticity. The derivation of this extension will be outlined. The new model combines both shallow water dynamics and classical water wave dynamics.
2. Luke's variational principle for classical water waves has been discretized using a discontinuous Galerkin finite element method. Preliminary numerical results will be presented.
3. Extensive tests have been performed for discontinuous Galerkin finite element shallow water models.

4. intend to outline a discretization based on the new variational principle, which satisfies the known limiting discretizations introduced above.
5. The final aim is to create a fast simulation tool for coastal dynamics with few degrees of freedom in the vertical but including accurate wave dispersion as well as shallow water dynamics.

## Room B3.02 Organiser: Charlie Elliott
## *Computational methods for interfaces and surfaces*

**Lubomir Banas** (Heriot-Watt) *Finite element approximation of a phase field model for multi-fluid incompressible magnetohydrodynamics*

We propose an implicit finite element method for a phase field approximation of time dependent multi-fluid incompressible magnetohydrodynamics. The proposed discretization satisfies a discrete energy law. We discuss computational aspects of the method and present some numerical experiments.

**Martin Rumpf** (Bonn) *Geodesics in shape space via variational time discretization*

A variational approach to defining geodesics in the space of implicitly described shapes is introduced in this paper. The proposed framework is based on the time discretization of a geodesic path as a sequence of pairwise matching problems, which is strictly invariant with respect to rigid body motions and ensures a 1-1 property of the induced flow in shape space. For decreasing time step size, the proposed model leads to the minimization of the actual geodesic length, where the Hessian of the pairwise matching energy reflects the chosen Riemannian metric on the shape space. Considering shapes as boundary contours, the proposed shape metric is identical to a physical dissipation in a viscous fluid model of optimal transportation. If the pairwise shape correspondence is replaced by the volume of the shape mismatch as a penalty functional, for decreasing time step size one obtains an additional optical flow term controlling the transport of the shape by the underlying motion field. The implementation of the proposed approach is based on a level set representation of shapes, which allows topological transitions along the geodesic path. For the spatial discretization a finite element approximation is employed both for the pairwise deformations and for the level set representation. The numerical relaxation of the energy is performed via an efficient multi-scale procedure in space and time. Examples for 2D and 3D shapes underline the effectiveness and robustness of the proposed approach.

**Bjorn Stinner** (Warwick) *On a surface finite element method for biomembranes with lipid decomposition*

Bilayers consisting of lipids molecules are the basic component of cell membranes. Vesicles formed from such biomembranes show a variety of interesting shapes that can be explained by its elastic bending energy. Due to inhomogeneities the lipids may separate and form different phases on the membrane which results in an energy contribution from the phase interfaces. We have been numerically studying equilibrium shapes, i.e., local energy minima by relaxing suitable initial shapes. A suitable (kind of) gradient flow dynamics has been defined for this purpose where the inter-membrane domains are described using the phase field methodology. The governing equations consist of pde on the membrane surface describing the phase separation coupled to a geometric evolution law for the membrane. The discretisation is based on representing the membrane by a triangulated surface on which quadratic parametric FEs are defined. The convergence as grid parameter and diffuse interface thickness tend to zero has been numerically investigated. Further issues are the sharp interface limit of the phase-field approach and adaptive mesh refinement.

**V Styles** (Sussex) *Primal-dual active set methods for Allen-Cahn variational inequalities*

We propose a primal-dual active set method for local and non-local Allen-Cahn variational inequalities. Properties of the method are discussed and numerical simulations are presented that demonstrate its efficiency.