Applied Maths Seminars 2016/17 Semester 1

5 October
SCH.1.05
2:00pm: Dr Zhong Zheng (Mechanical and Aerospace Engineering, Princeton University/visiting Cambridge)
Reduced-order Transport Models for Energy and the Environment

In this talk, I will discuss several reduced-order transport modeling studies motivated by energy and environmental problems: (i) Inspired by CO2 geological storage, we study fluid (CO2) injection into a confined porous reservoir initially saturated with another fluid (brine), and characterize the time evolution of the fluid-fluid (CO2-brine) interface. Because of the effect of confinement, we identify a transition from an early-time self-similar solution to three branches of late-time self-similar solutions for the interface shape. (ii) Inspired by shale gas recovery, we study the fluid-driven cracks in an elastic matrix and characterize the evolution of the crack shape; we also study the elasticity-driven backflow process following fluid injection, and obtain a simple scaling law for the backflow rate of the fracking fluids. (iii) I will also introduce our fundamental study on the viscous fingering instability, which is related to enhanced oil recovery, and report a series of time-dependent strategies for the stabilization of the viscous fingering instability at fluid-fluid (e.g., water-oil, gas-oil) interfaces. I will close the talk by discussing ideas for future exploration and collaboration.

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12 October
SCH.0.13
3:00pm: Dr Dan Lucas (DAMTP, Cambridge)
Instabilities, exact coherent structures and layer formation in horizontally shearing body-forced stably-stratified turbulence

We consider turbulence driven by a large scale horizontal shear by way of the Kolmogorov flow (sinusoidal body forcing) and a background linear stable stratification imposed in the third direction. This provides a tractable arena to investigate the formation of coherent structures, which in this case organise the flow into horizontal layers by inclining the background shear as the strength of the stratification is increased. By numerically converging exact steady states and continuing these new solutions in the control parameters, the coherent structures can be traced back to new instabilities of the base flow. We investigate how the vertical lengthscales observed in the turbulence are related to the instabilities and compare to the other well studied examples of instability driving layer formation. We also expose the chaotic motions of the stratified turbulence by locating unstable periodic orbits embedded therein.

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19 October
SCH.1.05
2:00pm: Professor Peter J. Larcombe (Dept. Computing and Mathematics, University of Derby)
Catalan Numbers and Catalan Polynomials: An Overview of Some Work in Discrete

Mathematics
Joint seminar with Geometry and Mathematical Physics

In this talk I will present some results from my work in discrete mathematics. Integer sequences whose (ordinary) generating functions satisfy a quadratic equation are common, and in any sequence instance the functional coefficients of the governing equation characterise a namesake family of polynomials. I will give some initial results for the general class of polynomials and then - in relation to the particular family of Catalan polynomials - present the algebraic execution of some numeric root finding schemes (including the classic Newton-Raphson and Halley algorithms) that are found to deliver non-linear polynomial identities; such identities - termed 'auto-identities', can be produced by computer for any polynomial family in the general polynomial class. On a different topic, it is found that a particular suite of trigonometric power series identities (whose origins date back to the some geometric models of the 17th century) provides fruitful ground for evaluations of sums of exponentiated multiples of Catalan number linear combinations - one or two different methods can be applied to achieve some pleasing results, and generalised.

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9 November
SCH.1.05
2:00pm: Dr Vasily Kostikov (Novosibirsk State University, Russia)
Unsteady free surface flow over a moving circular cylinder

A problem on non-stationary free surface flow of an infinitely deep ideal fluid generated due to the motion of a submerged body is considered. The initial formulation of the problem is reduced to an integral-differential system of equations for the functions defining the free surface shape, the normal and tangential components of velocity on the free boundary. Small- time asymptotic solution is constructed for the case of circular cylinder that moves with a constant acceleration from rest. The role of non-linearity is clarified by the analysis of this solution in the context of formation mechanism of added mass layers, splash jets and finite amplitude surface waves.

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16 November
SCH.1.05
2:00pm: Dr Ben Goddard (Maths, Edinburgh)
Dynamic Density Functional Theory: Modelling, Analysis and Numerics

In recent years, a number of dynamic density functional theories (DDFTs) have been developed to describe colloid particle dynamics. These DDFTs aim to overcome the high-dimensionality of systems with large numbers of particles by reducing to the dynamics of the one-body density, described by a PDE in only three spatial dimensions, independently of the number of particles. The standard derivations are via stochastic equations of motion, but there are fundamental differences in the underlying assumptions in each DDFT. I will begin by giving an overview of some DDFTs, highlighting the assumptions and range of applicability. Particular attention will be given to the inclusion of inertia and hydrodynamic interactions, both of which strongly influence non-equilibrium properties of the system. I will then demonstrate the very good agreement with the underlying stochastic dynamics for a wide range of systems. I will *also discuss an accurate and efficient numerical code, based on pseudospectral techniques, which is applicable both to the integro-PDEs of DDFT and to many other systems. Finally I will describe the rigorous passage to the high-friction limit, where the one-body density satisfies a nonlinear, non-local Smoluchowski-like equation with a novel diffusion tensor. I will also describe the (somewhat less rigorous) limit of being close to local equilibrium, in which we obtain a Navier-Stokes-like equation with additional non-local terms.*

Joint work with Serafim Kalliadasis, Greg Pavliotis, and Andreas Nold.

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1 December (Thursday)
SCH.0.13
3:00pm: Dr Diwei Zhou (Maths, Lboro)
Introduction to Statistics for Diffusion Tensor Imaging

Diffusion Tensor Imaging (DTI) is an advanced Magnetic Resonance Imaging (MRI) modality which provides unique insights into the microstructure and organisation of biological tissues in vivo and does so non-invasively. DTI has been applied to reveal subtle abnormalities in a large number of brain diseases and disorders including multiple sclerosis, stroke, schizophrenia, dyslexia etc. Also DTI has permitted researchers to investigate muscle structures. The central concept in DTI is the diffusion tensor. The geometric nature of the diffusion tensor can directionally and quantitatively capture the diffusion of water molecules in tissues such as white matter of the brain, cardiac muscles and skeletal muscles. Diffusion tensor processing must account for the diffusion tensor, which has a complicated mathematical structure, the three-dimensional spatial characteristics of the image, and the existence of complicated fibre structures in the biological tissues. The combination of these aspects makes diffusion tensor data calculation and DTI image processing one of the most challenging topics in the area of medical image analysis. The presentation will introduce what statistics can contribute to DTI data calculation and processing.

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7 December
SCH.1.05
2:00pm: Dr Georgy Kitavtsev (Applied Maths, Bristol)
Liquid crystal defects in the Landau-de Gennes theory in 2D-beyond the one-constant approximation

In this talk the two-dimensional Landau-de Gennes energy with several elastic constants, subject to general k-radial symmetric boundary conditions, will be analysed. It will be shown that for generic elastic constants the critical points consistent with the symmetry of the boundary conditions exist only in the case k=2. In this case one can identify three types of radial profiles: with two, three of full five components. Next, numerical results on domains of existence and stability of these radial solutions as well as of certain non-radial ones, so called two 1/2-defects solutions, will be collectively presented and discussed on the corresponding bifurcation diagrams in two cases: the usual case when the bulk energy vanishes on a uniaxial set of co-dimension 3, and degenerate one when it vanishes on a biaxial set of co-dimension 1.

Joint work with Jonathan Robbins, Valery Slastikov and Arghir Zarnescu.

Applied Maths Seminars 2016/17 Semester 2

Several UCAS visit days and other events occur in semester 2. Thus, seminars are not always regular. This semester a number of seminars are also run jointly with other relevant seminar series.

25 January
WPT006
2:00pm: Prof Moriarty (University of Nottingham)
Do we really see chemical bonds?
Landau seminar, Physics

Exceptionally clear images of intramolecular structure can now be attained in dynamic force microscopy (DFM) through the combination of tip-apex control and operation in what has become known as the "Pauli exclusion regime" of the tip-sample interaction [1-4]. (See, for example, Fig.1. This figure, taken from Ref. 4, shows a DFM image of a 2D assembly of NTCDI molecules alongside a ball-and-stick model of the molecule where blue spheres represent nitrogen atoms, and red spheres are oxygen.)

My particular focus will be on the interpretation of Pauli's principle in the context of interatomic and intermolecular interactions, what this means for the quantitative analysis of ultrahigh resolution force microscopy data, and whether or not we really see chemical bonds in DFM images [5,6].

[1] L Gross, et al., Science, 325 (2009) 1110
[2] Dimas G. de Oteyza, et al., Science, 340 (2013) 1434
[3] Jun Zhang, et al., Science 342 (2013) 611
[4] A Sweetman, et al., Nature Comm. 5 (2014) 3931
[5] P Hapala, et al., Phys Rev B 90, 085421 (2014); Sampsa K. Hämäläinen et al, Phys. Rev. Lett. 113, 186102 (2014)
[6] S. P. Jarvis, et al., Phys. Rev. B 92, 241405(R) (2015)

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1 February
SCH.0.01
3:00pm: Dr Timo Betcke (University College London)
Software frameworks for computational boundary element methods
Imaging Science, and joint Applied/Analysis seminar

In recent years Galerkin boundary element methods have become an important tool for large-scale simulations in bounded and unbounded homogeneous media. While the underlying mathematical theory is becoming more mature the development and implementation of fast and robust boundary element methods is still an active field of research. In this talk we present the BEM++ software framework for the solution of a range of boundary element problems from electrostatics, acoustics and computational electromagnetics. The guiding principle of BEM++ is to hide the implementational complexity by providing an interface that is as close to the mathematical description as possible. We will present the underlying ideas and theory and present a range of *interesting applications, in particular in acoustics and computational electromagnetics to demonstrate the design philosophy and capabilities of BEM++.*

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22 February
SCH.0.01
3:30pm: Prof Juan Carlos De los Reyes (Escuela Politécnica Nacional)
Learning optimal spatially-dependent regularization parameters in total variation image denoising
Imaging Science, and joint Applied/Analysis seminar

We propose a bilevel optimization approach in function space for the determination of the noise model and/or for the choice of spatially dependent regularization parameters in TV denoising models. The problems are treated as mathematical programs with partial differential variational inequality constraints and tailored regularization schemes for the approximation of the optimal parameters are proposed. Differentiability properties of the solution operator are studied. The optimal function values are numerically computed by using a combined Schwarz domain decomposition-semismooth Newton method applied to the optimality system. Exhaustive numerical computations are carried out to show the suitability of the approach.

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1 March
SCH.1.01
2:00pm: Prof Manolis Georgoulis (University of Leicester)
On space-time finite element methods for evolution PDEs

I review the problem of mesh design for numerical methods for (nonlinear) evolution PDEs, highlighting that without mesh modification a number of evolution PDE problems remain extremely challenging or even intractable. I will then move into proposing a new space-time finite element framework based on new, reduced-complexity, discontinuous Galerkin methods which aims to address nonlinear evolution problems through a combination of automatic mesh modification and modern mesh design techniques. After briefly discussing the new framework of reduced complexity discontinuous Galerkin methods for parabolic and second order hyperbolic problems, I will move on to the key question of incorporation of extremely general meshes, comprising of polygonal/polyhedral elements.

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29 March
SCH.1.01
2:00pm: Dr Mark Bankhead (National Nuclear Laboratory)
From modelling nuclear plants to the development of an Integrated Nuclear Digital Environment

Modelling and simulation are becoming ubiquitous in nuclear engineering driven by the increase in available computing power. At the same time the availability of sensors is increasing rapidly so that large amounts of data, known as ‘big data’, are being generated from both observations and simulations. New modelling approaches are *being developed which allow for more accurate physical descriptions of complex coupled phenomena allowing a phenomenological descriptions of the various processes involving radiation, chemistry, thermal and stress that could impact on the performance of a nuclear plant. Methods for assessing the impact of uncertainty on predictions have the potential to be used to integrate across broad spatial and temporal domains, from the microscopic forces in a small engineered component to an engineered nuclear system of plants and reactors. Finally, these approaches must be combined with a fundamental understanding of the governing mechanisms in order to maintain credibility with the industry regulators. This together represents a high level design concept of how virtual prototypes and digital twins can be combined to produce an integrated model of the lifecycle of a nuclear engineering system. Practical benefits in the real-world exist in today's problems for accelerating nuclear clean-up to tomorrow's problem of delivering safe, clean and sustainable nuclear energy in developed and emerging nations. Specific examples include the design of the next generation of nuclear fuels and the clean-up of nuclear facilities.*

Dr Mark Bankhead is a research chemist with over 15 years' experience working in the nuclear Industry with the National Nuclear Laboratory and its predecessor organisation. He is a technical specialist in quantum mechanical, atomistic and process plant modelling methods, with specific chemical expertise in the field of chemical reactivity at interfaces. He has applied these skills to address a diverse range of technical challenges across the nuclear fuel cycle including, heterogeneous catalytic reactions, corrosion chemistry, reactive transport and predictive modelling of materials performance. Since 2006, he has led High Performance Computing for NNL and is the lead in managing NNL's £0.5m HPC facility. He has authored a number of external peer reviewed scientific papers, several invited talks and conference articles and is the author of over 45 significant internal reports that have been subject to technical committee review. He is a visiting research associate with the University of Sheffield and the University of Liverpool where he is involved in the industrial supervision of a number of PhD projects across a range of technical areas.

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27 April (Thursday)
SCH.0.01
4:00pm: Prof Mikko Salo (University of Jyväskylä, Finland)
Inverse problems and imaging
Imaging Science, and joint Applied/Analysis seminar

This talk will give an overview of certain recent developments in the mathematical theory of inverse problems and related imaging methods, focusing on work carried out at the Finnish Centre of Excellence in Inverse Problems Research. We will discuss X-ray imaging, seismic imaging and diffuse imaging methods as well as related mathematical techniques from partial differential equations, differential geometry and integral geometry.

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10 May
SCH.1.01
2:00pm: Dr Ricardo Barros (Loughborough University)
Large amplitude internal waves in two- and three-layer flows

We revisit the strongly nonlinear long wave model for large amplitude internal waves in two-layer flows with a free surface proposed by Choi & Camassa (1996) and Barros, Gavrilyuk & Teshukov (2007). Its solitary-wave solutions are governed by a Hamiltonian system with two degrees of freedom, whose critical points are examined in detail leading to some new results. It will be shown how similar techniques can be used to study nonlinear internal waves in a three-layer flow confined between two rigid walls. Some preliminary results on mode-2 waves will be presented.

followed by

SCH.0.01
3:30pm: Dr Björn Sprungk (TU Chemnitz, Germany)
Metropolis-Hastings Algorithms for Bayesian Inference in Hilbert Spaces
(Joint with Analysis Seminar Series)

We consider Bayesian inference in Hilbert spaces, for example, inferring the uncertain diffusion coefficient in an elliptic PDE given noisy observations of the corresponding solution. To this end, we outline the Bayesian approach to inverse problems and discuss its well-posedness. In order to sample from the resulting posterior measure we will employ Markov Chain Monte Carlo methods. Here, we focus on Metropolis-Hastings (MH) algorithms.

These algorithms are usually easy to implement but their (statistical) efficiency often deteriorates if the (finite) state space dimension increases or if the posterior measure itself becomes more concentrated, e.g., due to more accurate observational data. This talk addresses techniques to circumvent these problems.

First, we describe how to define MH algorithms in infinite-dimensional Hilbert spaces and how this may yield a dimension-independent performance. In addition, we explain how to exploit information about the posterior covariance in order to construct more efficient MH algorithms which may even show a robust performance w.r.t. concentration of the posterior measure or the data accuracy, respectively.

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12 May (Friday)
SMB.0.02
3:30pm: Prof Dr Dirk Lorenz (Braunschweig)
Variational methods and optimization in imaging
Imaging Science, and joint Applied/Analysis seminar

Many tasks in imaging can be formulated as variational problems, i.e. as problems where some functional has to be minimized. Two main questions are:
1) How to formulate a good objective function such that we can expect the minimizers to have the desired properties?
2) How to compute a minimizer of the objective functionals?
Since in many cases the object of interest is an image, the number of variables of the objective function is usually in the order of the number of pixels. Hence, the minimization task is often a significant challenge. We see that both questions are somehow intertwined: One should design the objective function in a way that the resulting problem can be tackled by some numerical method.

23 May (Tuesday)
SCH.0.01
1:00pm: Michelle Maiden (University of Colorado, Boulder)
Nonlinear modulated wavetrains in viscous fluid conduits

Viscous fluid conduits provide an ideal system for the study of dissipationless, dispersive hydrodynamics. A dense, viscous fluid serves as the background medium through which a lighter, less viscous fluid buoyantly rises. If the interior fluid is continuously injected, a deformable pipe forms. The long wave interfacial dynamics are well-described by a dispersive nonlinear partial differential equation. In this talk, experiments, numerics, and asymptotics of the viscous fluid conduit system will be presented. Structures at multiple length scales are discussed, including solitons, dispersive shock waves, and periodic waves.

Experiments involving solitons, wavebreaking leading to dispersive shock waves (DSWs), and their interactions will be presented. The results include the refraction and absorption of a soliton by a DSW and the refraction of a DSW by a second DSW, resulting in two-phase behavior. Excellent agreement between nonlinear wave (Whitham) averaging, numerics, and laboratory experiments will be presented.

Modulations of periodic waves will be explored in the weakly nonlinear regime with the Nonlinear Schrödinger (NLS) equation. Modulational instability (stability) is identified for sufficiently short (long) periodic waves due to a change in dispersion curvature. These asymptotic results are confirmed by numerical simulations of perturbed nonlinear periodic wave solutions. Also, numerically observed are envelope bright and dark solitons well approximated by NLS.

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24 May
SCH.1.01
2:00pm: Dr Halim Kusumaatmaja (Durham)
Modelling Drop Motion and Contact Line Dynamics Using Diffuse Interface Models

I will discuss two applications of diffuse interface models for studying wetting and interfacial dynamics. In the first part of the talk, I will show how we can reconcile two scaling laws that have been proposed in the literature for the slip length associated with a moving contact line in diffuse interface models, by demonstrating each to apply in a different regime of the ratio of the microscopic interfacial width and the macroscopic diffusive length. The latter depends on the fluid viscosity and the mobility governing intermolecular diffusion. I also give evidence that modifying the microscopic interfacial terms in the model’s free energy functional appears to affect the value of the slip length only in the diffuse interface regime, consistent with the slip length depending only on macroscopic variables in the sharp interface regime. In the second part of the talk, I will discuss how to generalise diffuse interface models to account for an arbitrary number of fluid components, including introducing high density ratios between the fluid components. I will then highlight how such a model can be exploited to study droplet motions on liquid infused surfaces. These are liquid repellent surfaces made by infusing a lubricant into porous or rough solid surfaces.

2 June (Friday)
SCH.0.01
2:00pm: Prof Victor Shrira (Keele)
Kinetic equations vs direct numerical simulations of weakly nonlinear random wave fields: What is wrong with the kinetic equations?

The challenge of describing evolution of random weakly nonlinear dispersive waves in fluids and solids in various contexts is a major open fundamental problem despite being intensively studied theoretically and experimentally for more than fifty years. In contrast to the classical hydrodynamic turbulence, there is a well-established general formalism for treating weakly nonlinear wave fields that exploits smallness of nonlinearity and subtle assumptions about quasi-Gaussianity of a statistically homogeneous wave field. This approach leads to a closed equation for the second statistical momenta of the field which we will refer to as the kinetic equation} (KE). Although the theory based upon the KE has been able to predict the major features of wave field evolution (e.g. [3]) and is widely used (e.g. [1,2]). However the basic question --- to what extent the theory captures the actual behaviour of the wave field --- remains open. Here we address it by performing a detailed comparison of predictions of the KE and its generalization (gKE) with the results of direct numerical simulations (DNS) employing the algorithm specially designed for long term evolution of random weakly nonlinear wave fields. For certainty and without much loss of generality we perform these comparisons for weakly nonlinear water waves.

We take as the starting point the equations of motion in the form of the "four-wave" Zakharov equation without forcing. The KE and gKE are both derived from the this Zakharov equation under an assumption of weak non-Gausianity of the wave field and a closure hypothesis for the field higher statistical moments. We simulate numerically long-term evolution of wave spectra without forcing using three different models: (i) the classical kinetic equation (KE); (ii) the generalised kinetic equation (gKE) valid also when the wave spectrum is changing rapidly; (iii) the DNS based on the Zakharov integrodifferential equation for water wave which does not rely on any statistical assumptions. All three approaches demonstrate very close evolution of integral characteristics of spectra. Theoretically predicted regimes and asympotics do occur. However, there are substantial systematic differences (e.g. the broadening of angular spectra is much faster for the kinetic equations, the shape of the spectra are also noticeably different), which suggests the presence and significance of coherent interactions not accounted for by the established closure for the kinetic equations. This implies that the fundamental issue of closure for random wave fields has to be revisited.

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26 July
SMB.0.17
2:00pm: Prof Irina V. Semenova (The Ioffe Institute of the Russian Academy of Sciences)
Experimental observations of bulk strain soliton formation and evolutio