SIAM Chapter Day, Cardiff University, UK

School of Mathematics, Senghennydd Road, Cardiff, CF24 4AG, Wales

January 21, 2013

PROGRAMME

11:00 - 11:10 Introduction and Welcome

11:10 - 12:00 Nick Higham
Accuracy and Stability of Numerical Algorithms

12:10 - 13:00 Alain Goriely
Inversion, Rotation, and Perversion in Mechanical Biology: From Microscopic Anisotropy to Macroscopic Chirality

13:00 - 14:00 Posters Presentation and Lunch in Room M1/02

14:10 - 15:00 Simon Cox
Bubble-Scale Predictions of How Foams Flow

15:10 - 16:00 Matthew Gilbert
Application of Layout Optimization to Engineering Analysis and Design Problems

16:00 - 17:00 Concluding Discussions over Tea, Coffee, and Welsh Cakes in Room M1/02

All lectures will take place in Room M0/40, School of Mathematics, and will be co-chaired by Chris Rowlatt (President of SIAM Student Chapter) and Olivier Goury (Vice-President of SIAM Student Chapter).

ABSTRACTS OF LECTURES

Accuracy and Stability of Numerical Algorithms

Nicholas J. Higham

School of Mathematics, University of Manchester, Manchester, M13 9PL, England
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We discuss a number of issues concerning the behaviour of numerical algorithms in finite precision arithmetic. Specific topics to be addressed include

- How to reformulate expressions to allow more accurate evaluation, including by use of the unwinding number.
- The need for, and exploitation of, higher precision (e.g., quadruple precision) arithmetic.
- Abnormally small relative errors and their effects on performance profiles.

The talk will be accessible to those who are not specialists in numerical analysis.

Inversion, Rotation, and Perversion in Mechanical Biology: From Microscopic Anisotropy to Macroscopic Chirality

Alain Goriely

Mathematical Institute, University of Oxford, Oxford, OX1 3LB, England
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One of the fundamental problems of mechanical biology is to understand the relationship between a microscopic structure and its overall macroscopic response. A paradigm for this problem is chirality. How does a right-handed structure behaves under loads? How is chirality transferred between scales. The simplest example motivated by the study of DNA is the extension of a right-handed spring under pure axial load. Would it rotate clockwise or counter-clockwise? Similarly, many plant structures are fibre-reinforced and an outstanding problem is to connect the cell wall chirality with the chirality of the rotation induced by change in pressure. Motivated by different biological experiments on active gels, DNA, plant cell walls, and fungi, I will show that biological systems, through a combination of internal stresses and nonlinear responses offer many puzzling and often counter-intuitive chiral behaviours leading to the interesting possibility of perversion, an inversion in chirality under loads or remodeling. Based on these ideas, I will also develop a general mathematical framework to understand non-monotonous response of nonlinear materials.

Bubble-Scale Predictions of How Foams Flow

Simon Cox

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Foams are used in many ways: industrially they enable enhanced oil extraction from porous media and ore separation in mining, while domestically they are important in foods and cosmetic products. Being able to predict their behaviour under a given perturbation stimulates improved efficiency of industrial processes and the possibility to relate chemical formulation to rheology and hence to consumer satisfaction.

Foam structure is disordered but not disorganized. I will describe the bubble-scale structure, and show how it can be used as the basis for modelling the flow of foams. In particular, I will give examples of confined flows and the emerging field of discrete microfluidics in which foams are pushed through narrow channels. Correctly modelling the dissipation mechanisms and developing an accurate numerical algorithm is required to predict the material response.

Application of Layout Optimization to Engineering Analysis and Design Problems

Matthew Gilbert

Department of Civil and Structural Engineering, University of Sheffield, Sheffield, S1 3JD, England
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To verify the safety of solid bodies and structures against collapse, engineers have traditionally had to rely either on simplistic hand type calculations, or on significantly more complex computational tools which identify the collapse state in an indirect, iterative, manner (which can be costly in terms of computer and/or operator time). Additionally, in many engineering disciplines the initial design stage is carried out in an ad-hoc manner, with engineering intuition often used to identify structurally efficient designs. Direct analysis and design methods can potentially address both these issues, and similarities between analysis and design formulations can also potentially be exploited. Here the so-called layout optimization technique is described, and then applied to truss design problems and to the problem of identifying the critical layout of slip-line discontinuities in a solid body at the point of collapse. In each case mathematical programming techniques are used to obtain highly accurate solutions. Future directions in the field of layout optimization are then briefly considered.

LIST OF POSTERS

1. Numerical modeling of hydraulic crack propagation - Various leak off regimes

   Piotr Kusmierczyk, Institute of Mathematics and Physics, Aberystwyth University

   - PKN model is reformulated with newly introduced findings;
   - Alternative Problem variables are presented;
   - MATLAB based solvers and their accuracy is discussed.

2. Mathematical modelling of piezoelectric actuators using bimaterial interfaces

   Lewis Pryce, Institute of Mathematics and Physics, Aberystwyth University

   - Piezoelectric materials and the mathematical equations associated with them are introduced;
   - Piezoelectric actuators are related to problems concerning interfacial crack propagation;
   - Prior results for a semi-infinite crack propagating at a constant speed along a perfect interface between anisotropic materials are reviewed;
   - The roles of weight functions and the Betti formula in deriving stress intensity factors and second order asymptotic terms for arbitrary loading on the crack faces are discussed;
   - Numerical results for a given asymmetric loading system are presented.

3. The matrix unwinding function

   Mary Aprahamian, School of Mathematics, University of Manchester

   - A new primary matrix function arising from the multivalued nature of well-know complex functions, such as the logarithm and square root, is presented;
   - We use this to recover many mathematical identities trivially true in the real case and failing in the complex case;
   - We also introduce an idea of argument reduction for computing the matrix exponential and trigonometric function which relies on the unwinding function.

4. Computing the matrix logarithm and its condition number

   Samuel Relton, School of Mathematics, University of Manchester

   - New algorithm for efficient computation of the matrix logarithm in real arithmetic;
   - New algorithm for computation of the derivatives and condition number of the logarithm;
   - Performs better than existing methods in terms of both speed and accuracy.

5. Coupled magneto-mechanical-fluid simulation using *hp* finite elements

   Darong Jin, College of Engineering, Swansea University

   - Coupled solution of magneto-mechanical-fluid problems using a consistent Newton-Raphson linearisation and an *hp*-finite element discretisation;
   - Applications to 2D Navier-Stokes fluids, 2D magnetostrictive fluids and 2D magnetohydrodynamics;
   - Appropriate compatible discretisations, satisfying LBB conditions, are applied;
   - Efficient vectorised MATLAB implementations;
   - Convergence studies and benchmarking undertaken.

6. An eXtended spectral element method for two-phase viscoelastic flows

   Chris Rowlatt, School of Mathematics, Cardiff University

   - Description of the eXtended Spectral Element Method (XSEM) is given;
   - Comparison between SEM and XSEM is presented for a one-phase incompressible Oldroyd-B fluid with an immersed membrane/interface, where only the pressure solution is enriched;
   - Preliminary results for an incompressible Oldroyd-B fluid with discontinuous solvent viscosity are also presented.

7. Numerical simulations of collapsing toroidal bubbles with biomedical applications

   Mike Walters, School of Mathematics, Cardiff University

   - The Boundary Element Method (BEM) is used to model bubble collapse in the vicinity of a rigid wall;
   - Two extensions of this method to model toroidal bubbles are presented and compared.

8. The cure to the curse of dimensionality?

   Tom Croft, School of Mathematics, Cardiff University

   - An efficient method for solving problems defined in high dimensional domains is sought;
   - A Proper Generalised Decomposition (PGD) algorithm is proposed which provides a drastic reduction in degrees of freedom for high dimensional problems;
   - Convergence results are provided for the Poisson equation by comparison with greedy algorithms from nonlinear approximation theory;
   - Future work into PGD algorithms based on least squares formulations is proposed with the expectation to extend convergence proofs to a larger class of problem.

9. Solving differential algebraic equations by structural analysis - figures on numerics and structure

   Ross McKenzie, School of Mathematics, Cardiff University

   - An overview of the structural analysis (SA) method for differential algebraic equations (DAEs) is given;
   - The SA method is applied to the simple pendulum DAE with varying accuracies;
   - An analysis of the space of different offset vectors for a DAE with some examples is also presented.

10. Rationalising the computational expense in multiscale fracture mechanics: partitioned proper orthogonal decomposition

    Olivier Goury, **Pierre Kerfriden**, **Stéphane Bordas**, School of Engineering, Cardiff University

    - A coupling of domain decomposition and projection-based model order reduction is used to significantly reduce the computational time of a large nonlinear finite element simulation whilst keeping accuracy;
    - Applications can range from surgical simulations to advanced early-stage design in aeronautics.

11. Increased reliability for industrially relevant automatic crack growth simulation with the eXtended finite element method

    Octavio Andrés González Estrada, **Danas Sutula**, **Cheng-Kye Lee**, **Pierre Kerfriden**, **Stéphane Bordas**, School of Engineering, Cardiff University

    - We simulate the growth and interaction of multiple cracks using XFEM;
    - Smoothed FEM (SFEM) can deal with locking problems effectively with the strain smoothing in both linear and nonlinear elasticity.

12. More with less in computational mechanics

    Stéphane Bordas, **Pierre Kerfriden**, **Ahmad Akbari**, **Daniel Alves Paladim**, School of Engineering, Cardiff University

    - We provide more information for less computational expense to engineers and scientists by implementing advance numerical techniques;
    - XFEM is used to avoid remeshing the domain of study in the presence of moving boundaries, e.g. crack;
    - Homogenization technique: to use microscopic details in a macroscopic problem.

13. GPU-based Algorithms for cutting deformable objects in implicit simulations

    Hadrien Courtecuisse (a), **Pierre Kerfriden** (a) , **Christian Duriez** (b), **Jérémie Allard** (b), **Stéphane Cotin** (b), **Stéphane Bordas** (a), a: Cardiff University, UK, b: Inria Lille, France

    - We present a series of contributions in the field of real-time simulation of soft tissue biomechanics;
    - These contributions are based on the FEM Corotational model, and we rely on GPU implementations to enable real time computations.