



HPC/NA Workshop 1: Applications: underlying algorithms and challenges for the future

Oxford e-Research Centre

Day 1: Wednesday 5th November

- 11:00 Welcome
Introductions & aims of workshop by Anne Trefethen, OERC
Morning Sessions chaired by Iain Duff, STFC
- 11:15-13:15 **Large Scale Simulation**
- Stewart Cant, Cambridge
 - Leigh Lapworth, Rolls Royce
 - Wayne Arter, UKAE
 - Tom Theuns, Durham
- Group discussions
- 13:15-14:00 Lunch
Afternoon Sessions Chaired by Nick Higham, Manchester
- 14:00-15:30 **Biomedical Simulation**
- Nic Smith, Oxford
 - Mark Sansom, Oxford
- Group Discussions
- 15:30-17:30 **Computation for Physical Sciences Session I**
- Ken Taylor, QuB
 - Ilya Kuprov, Durham
 - Ivan Graham & Robert Scheichl, Bath
- Group Discussions
- 17:30-18:00 Plenary review & discussion of first sessions
- 18:30 Pre-dinner drinks, St. Hugh's College
- 19:00 Dinner, Wordsworth Room, St Hugh's College

Day 2: Thursday 6th November

- 09:00 Welcome to the workshop & summary by Anne Trefethen, OeRC
Morning Sessions Chaired by Iain Duff, STFC
- 09:30-10:45 **Computational Finance**
- Mike Giles, Oxford
- Group Discussions
- 11:30-13:00 **Computation for Physical Sciences II**
- Chris Goodyer, Leeds
 - Björn Stinner, Warwick
 - Ian Bush, NAG
- Group Discussions
- 13:00-14:00 Lunch
Afternoon Sessions chaired by Anne Trefethen, OeRC
- 14:00-16:00 **Oceanography and Climate Modelling**
- Gerard Gorman, Imperial
- Group Discussions
- 16:30-17:30 Review & discussion of day 2
- 18:30 Pre-dinner drinks, St. Hugh's College
- 19:00 Dinner, The Boardroom, St Hugh's College

Day 3: Friday 7th November

- 09:00 Welcome to the workshop & summary by Anne Trefethen, OeRC
Morning Sessions chaired by Nick Higham, Manchester



09:30-11:30	Computation for Physical Sciences Session III <ul style="list-style-type: none">• Tony Arber, Warwick (Physics)• Paul Sherwood (Comp Chem)• Cliff Addison, Liverpool Group discussions
11:30-12:30	Review of workshop and outputs
12:30-13:30	Lunch
	Discussion – first thoughts for roadmap
	Plans for second workshop, Manchester December 2008
15:00	Close



Speaker Details

Stewart Cant, Department of Engineering, Cambridge

Algorithms for computational fluid dynamics

Leigh Lapworth, Rolls Royce

HPC - The Challenges of Gas Turbine Engines

Brief 10 minute overview of some of the simulation challenges posed by Gas Turbine engines, such as virtual engine, multi-physics, etc.

Wayne Arter, EURATOM/UKAEA Fusion Association, Culham Science Centre

Fusion plasmas have been extensively modelled using fluid models, historically MHD models (coupling to a co-evolving magnetic field) in relatively simple toroidal geometry. There is therefore interest in algorithms which take forward both compressible and incompressible hydrodynamics. However, numerical simulation of fusion plasmas is now increasingly taking into account velocity-space effects, ie. using models based on the Vlasov/Boltzmann equation, and therefore algorithm development for 5D/6D problems coupled to Maxwell's equations would be of interest. This includes both particle simulation, where fast algorithms for particle tracking/ray-tracing would be helpful and gyrokinetics (fully mesh-based) simulation where better preconditioners are required. Multi-dimensional Fourier transforms are relevant to both cases. This work was funded jointly by the United Kingdom Engineering and Physical Sciences Research Council and by the European Communities under the Contract of Association between EURATOM and UKAEA.

Tom Theuns, Institute of Computational Cosmology, Durham

Cosmological simulations of galaxy formation: techniques and their implementation

Nic Smith, Computing Laboratory, Oxford

My research program is characterised by the development of integrated multi-scale and multi-physics models primarily of the heart which provide the ability to link biophysically detailed experimental and clinical data to integrated function from sub-cellular to whole organ level. Within the scope of this work I am interested in developed computational techniques to enable model development and specific models to provide insight into cardiac physiology. This work is focused on cardiac electrophysiology and contraction at the cellular level and the multi-scale translation of these models to simulate blood flow and cardiac electro-mechanics at the tissue level. The application of these models to understand the mechanisms of underlying coronary artery disease and heart failure to assist the development of new treatments and guide existing therapies is the ultimate goal of this work.

Mark Sansom, Structural Bioinformatics and Computational Biochemistry Unit, Oxford

The overall theme of work in my group is to employ a range of computational techniques (structural bioinformatics, molecular modelling, MD simulations, etc.) to membrane proteins.



Ken Taylor, Queens University Belfast

Solving time-dependent high-dimensional linear PDEs on MPP architectures

On large-scale MPP architectures minimization of inter-processor communication is one of the most important goals. In our own problem domain we have an additional requirement for very high accuracy. We discuss how these two constraints can be met by the use of high-order explicit propagators. We illustrate their use in handling a high-dimensional form of the Schroedinger equation on machines such as the Cray XT4, where a high degree of scalability has been achieved. This has made possible the solution of previously intractable problems.

Ilya Kuprov, Chemistry Department, Durham

Computational problems of spin dynamics: from sparse matrices to cancer diagnostics

The presentation will focus on current computational problems in Physical and Theoretical Chemistry and will attempt to describe the challenges encountered in that field within the Computational Science framework. Specifically, the talk will focus on the common bottlenecks (matrix diagonalization, matrix exponentials, computational scaling) encountered in Theoretical Chemistry calculations, their context and possible strategies of eliminating them.

Ivan Graham and Robert Scheichl, Mathematical Sciences, Bath

Future algorithm and software development in industrial applications of PDEs

In this talk we highlight current research and future algorithmic requirements in several classes of problems involving applications of partial differential equations. These include: (i) Uncertainty quantification problems arising in radioactive waste disposal, groundwater flow and climate modelling; (ii) Sensitivity and criticality analyses in fluid flow and in nuclear reactor simulation; (iii) Modelling of heterogeneous media and high frequency scattering. Key algorithmic/software requirements include the treatment of very high-dimensional problems, sparse solvers for discrete systems of PDEs in 3D, robust iterative eigenvalue solvers for complex applications and fast iterative methods for dense systems.

Mike Giles, Mathematical Institute, Oxford

Computational finance

I will give an overview of the main numerical methods used in computational finance, and discuss the HPC needs which have made this area arguably the largest HPC user in the UK.

Christopher Goodyer, School of Computing, Leeds

This talk will briefly summarise the HPC work of the Scientific Computation group in the School of Computing at the University of Leeds. The focus will be on three parallel applications, namely lubrication modelling, phase-field modelling and simulation of chemical diffusion through skin. We will also look forward to the future advances needed in development of efficient algorithms for evolving computational technologies.



Björn Stinner, Warwick Mathematics Institute, University of Warwick

PDEs on moving surfaces - computational issues

We consider free boundary problems with quantities located on the moving surfaces which are subject to PDEs. Different representations of the free boundaries - moving hypersurfaces, thin interfacial layers etc. - require different approaches for the surface quantities. To motivate the computational issues associated with these approaches, exemplary, we will focus on surfactants in two-phase flow and relaxational dynamics of elastic biomembranes with lateral phase separation. In the first example, a Navier-Stokes system is coupled to a Cahn-Hilliard equation for the phase interface motion. Using P2/P1 finite elements for the fluid flow equations results in a saddle point problem to be solved in each time step, which is done with a preconditioned GMRES. The fourth order interface equation can be split into two second order problems for which we used P1 FE. The use of obstacle potentials leads to variational inequalities that have been solved so far based on a Gauss-Seidel type iteration. A surfactant altering the surface tension and subject to an advection diffusion equation along the phase interface can be approximated by P1 FE as well. Solving with a preconditioned CG variant this part of the problem is rather cheap. In the second example, the energy of a biomembrane consists of elastic contributions and contributions arising from lipids separating along the surface. To compute equilibrium shapes a gradient flow dynamics has been set up resulting in a parabolic fourth order equation for the membrane motion. Second order splitting and using parametric P1 surface FE leads to a discrete system of linear equations solved so far by a CG variant. It is desirable to apply more regular FE spaces leading to more off-diagonal entries.

Ian Bush, NAG Ltd

Computational Materials Science

Gerard Gorman, Applied Modelling & Computation Group, Imperial

Model development work for the Imperial College Ocean Model.

Tony Arber, Centre for Fusion, Space and Astrophysics, Warwick

Computational Plasma Physics

A summary of the computational challenges facing plasma physics with particular emphasis on laser plasmas, fusion and space physics.

Paul Sherwood, STFC

Numerical Algorithms for Computational Chemistry

I will review the use of numerical libraries in quantum chemistry and molecular dynamics applications, considering the performance bottlenecks on serial and parallel hardware.

Cliff Addison, Liverpool



I will discuss our experiences getting applications to run well on Barcelona systems. We have seen some mixed results (dense matrix xhpl extremely good, the ab initio molecular modelling code VASP - scaling issues with multiple cores per node).