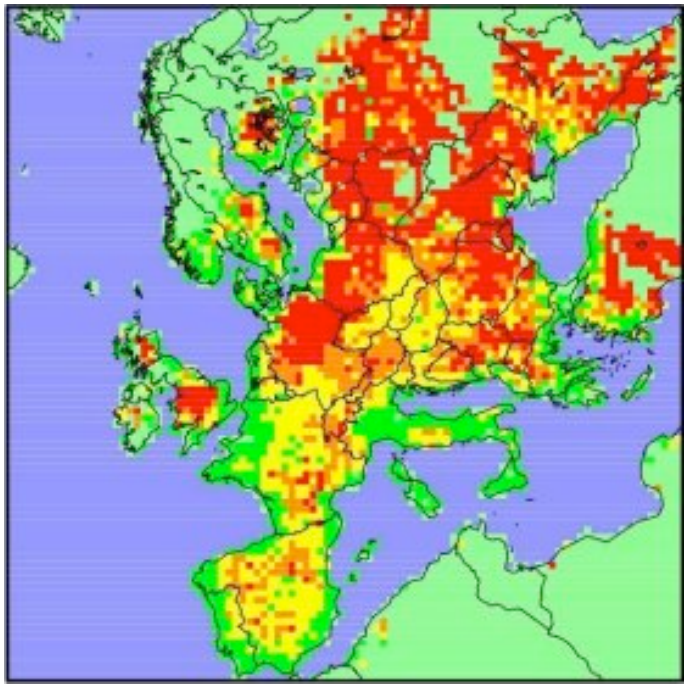
Second Reading Workshop on Computational Sciences



Organised by ACET

School of Systems Engineering
Philip Lyle Building

11^{th} December 2006

University of Reading

Purpose: To define the roadmap for Computational Science at Reading for the next four years.

Focus on: Modelling of Complex Systems, Scalable Algorithms, Tools and Environments for Wide Area Distributed Computing.

Contents

Programme

9:30 - 9:45	Introduction by *Prof. Vassil Alexandrov*
9:45 - 10:30	Invited talk by *Prof. Zahari Zlatev*, National Environmental Research Institute, Denmark
10:30 - 11:30	Talks (15 minutes each): *Cihan Sahin*, ACET Centre *Prof. Ivan Dimov*, ACET Centre *Prof. Rainer Cramer*, Director, BioCentre *Dr. Kimberly Watson*, Structural Biology, BioCentre
11:30 - 12:00	Coffee/Tea
12:00 - 13:00	Talks (15 minutes each): *Dr. Andrew Meade*, Computational Biology, AMS *Dr. Amos Lawless*, Mathematics and DARC *Prof. Mike Baines*, Mathematics *Prof. Simon Chandler-Wilde*, Mathematics
13:00 - 14:00	Lunch
14:00 - 15:00	Discussion and Coffee/Tea

Prof. Zahari Zlatev

Treatment of Comprehensive Environmental Models

Exceeded critical levels of the environmental pollution may cause different damages on eco-systems, vegetables, animals and, what is perhaps most important, on human health. Comprehensive mathematical models can successfully be used in order to find out whether some critical levels of the environmental pollution (for example, critical levels established in the European Union) are exceeded or not. It is normally required to calculate more detailed and more reliable results. This leads to huge computational tasks. In order to able to resolve efficiently these tasks it is necessary to:

- to implement fast and sufficiently accurate numerical algorithms,
- to reorganize the computations in order to exploit better the cache memories of the modern computers and
- to develop parallel codes.

The treatment of these tasks will be discussed in this talk. The solution of these problems is based on ideas presented in Alexandrov et al. [1] and Zlatev and Dimov [3]. As an illustration some results obtained when the impact of climatic changes on the pollution levels in Europe (Zlatev et al. [2]) will be presented.

[1] V. N. Alexandrov, W. Owczarz, P. G. Thomsen and Z. Zlatev: "Parallel runs of a large air pollution model on a grid of Sun computers". Mathematics and Computers in Simulation Vol. 65 (2004), pp. 557-577.
[2] P. Csomos, R. Cuciureanu, G. Dimitriu, I. Dimov, A. Doroshenko, I. Farago, K. Georgiev, A. Havasi, R. Horvath, S. Margenov, L. Moseholm, Tz. Ostromsky, V. Prusov, D. Syrakov and Z. Zlatev: "Impact of Climate Changes on Pollution Levels in Europe",
`http://www.rdg.ac.uk/~sis04itd/MyPapers/climatic_scenarios_NATO.pdf`.
[3] Z. Zlatev and I. Dimov: "Computational and Numerical Challenges in Environmental Modelling", Studies in Computational Mathematics, Vol. 13, Elsevier Science, Amsterdam, 2006.

Bio

http://www2.dmu.dk/atmosphericenvironment/staff/zlatev.htm

Prof. Vassil Alexandrov

Abstract

Bio

Vassil Alexandrov is a Professor in Computational Sciences at the School of Systems Engineering, Director of the Centre for Advanced Computing and Emerging Technologies and Head of Research of PEDAL Laboratory at the University of Reading, UK. He has obtained his MSc in Applied Mathematics from Moscow State University in 1984 and his PhD in parallel computing from the Institute for Parallel Processing at the Bulgarian Academy of Sciences in 1995.

His main interests are in the area of simulation and modelling of complex systems, parallel scalable algorithms, Collaborative, Cluster and Grid Computing and using the advances in the above mentioned areas for efficiently solving large scale scientific and industrial problems. He is currently participating in over 6 national and international projects in the area of Collaborative and Grid Computing and e-learning. He also collaborates with Intel and IBM in the areas of Collaborative and High End Computing and with Oak Ridge National Laboratory, Supercomputing Centre in Barcelona, Daresbury Laboratory, IPP - Sofia, SZTAKI - Budapest, Emory University and University of Tennessee in the area of Collaborative, Cluster and Grid computing.

Cihan Sahin

Performance Analysis of a Large Scale Environmental Model on ACETs BladeCenter

Many complex scientific software need to be ported and performance tuned to different platforms as more supercomputers and clusters become available to scientific community. This talk looks at the porting and performance analysis of a Unified Large Scale Air Pollution Model (UNI-DEM), developed by the Danish National Environmental Research Institute, to a large cluster system (A Blade cluster, BC). As UNI-DEM has been developed and tested on smaller clusters, enabling the UNI-DEM on larger clusters, typically bigger then 100 processors, is of interest especially from the point of performance. Tehcnical problems asscoiated on porting procedure is also identified and solved. Multiple parallel runs with different configurations are carried out to analyse the scalibility hence the performance of the code on BC architecture.

Bio

Cihan Sahin is a Phd student at School of Systems Engineering, The University of Reading, and a member of the Advanced Computing and Emerging Technologies (ACET) Research Group. His main research interests are parallel applications and grid computing. He is currently working on the development of a grid interface for Unified Air Pollution Model (UNI-DEM).

Prior to his PhD studies, he gained a MSc degree in Network Centred Computing from the University of Reading in 2005. He also works for ECMWF as a programmer.

Prof. Ivan Dimov

Robustness of Markov Chain Monte Carlo for Very Large Linear Algebra Problems

A Markov chain Monte Carlo algorithm for very large Linear Algebra Problems will be presented. In our consideration, "very large" matrix means dense or unstructured general sparse matrix with a number of non-zero entrances ranging from one million to one billion. The concept of robustness for stochastic algorithms is introduced. We analyse the robustness theoretically and numerically for both kinds of matrices – dense and sparse. Numerical experiments with different very large matrices will be analysed from both points of view: accuracy of the method and performance of the algorithm.

Bio

Professional Experiences:
Monte Carlo solution of partial differential equation, a priori estimates and error analysis; statistical numerical methods with supper convergent probability error; parallel algorithms and Grids; and mathematical modelling and scientific computation in environmental mathematics, gas discharge plasma, and semi-conductors physics.

Doctor's Degrees:
PhD in Mathematical modelling - Moscow, Russia (1980). DSc in Numerical Analysis - Moscow, Russia (1984).

Professional Record:
Researcher in Numerical Analysis (1982-1985) and Associate Professor in Numerical Analysis (1985-1990) at the Institute of Mathematics, Bulgarian Academy of Sciences, Sofia, Bulgaria. Associate Professor in Parallel Algorithms, Head of the Laboratory of High-Performance Systems and Parallel Algorithms, Deputy Director of the Center for Informatics and Computer Technology, Bulgarian Academy of Sciences (1990-1995). Professor in Mathematical Modelling (1996-), and Director of the Institute for Parallel Processing (1996-2004), Bulgarian Academy of Sciences. Head of the Bulgarian Information Society Centre of Excellence for Education, Science and Technology in 21 Century (BIS-21), Bulgaria (2000-). President of Scientific Council of IPP-Bulgarian Academy of Sciences (2004-). Research Professor, ACET Centre, The University of Reading, UK (2005-).

Prof. Rainer Cramer

SPEEK - Systems Biology at Reading - Abstract

Systems biology (SB) aims for the comprehensive description of complex biological systems. One central objective within SB is to derive predictive models of cell functionality, and a number of projects around the world are already addressing this using microbial and eukaryotic cell systems. We have proposed a five-year project taking one of the simplest functional eukaryotic cell types, the platelet, and to examine how its behaviour and function is determined by its easily sampled environment – the blood.

Bio

Professor Cramer joined the University in January 2005 as the Director of the BioCentre and Professor of Mass Spectrometry and Bioanalytical Sciences in the School of Chemistry.

He obtained his doctoral degree in Prof Hillenkamp's laboratory, the birthplace of matrix-assisted laser desorption/ionization (MALDI), which together with electrospray ionization (ESI) is the main technique in modern biological mass spectrometry (MS). He joined the Ludwig Institute of Cancer Research in 1997 and became an Assistant Member and the Head of Bioanalytical Chemistry in 1999. He is also affiliated with UCL and is currently Reader in Biological Mass Spectrometry in their Department of Biochemistry.

Dr Cramer is a truly interdisciplinary researcher, who started his academic career as an experimental physicist and later moved on to cancer research and other research fields in the life sciences. He has a strong background in proteomics, biological mass spectrometry and analytical chemistry. In general, his research interests are built around the application of his physical science expertise to the analytical challenges posed by modern biosciences.

Dr. Kimberly Watson

Bio

Kimberly Watson is Head of The Structural Biology Unit. Her research areas are Protein Structure & Function and Plant Biochemistry & Physiology.

Type II diabetes (non-insulin dependent) is a familial disease affecting approximately 8% of the UK population aged 60-69 years. The problem of maintaining good glycaemic control can be approached through an understanding of proteins involved in glycogen metabolism and insulin secretion. Her group is using X-ray crystallography, various biophysical methods, and computational approaches to study the structure and function of the targets that play a role in glucose homeostasis in an effort to develop more effect therapeutic treatments for diabetes.

Currently, their studies are focused on proteins involved in liver and muscle glycogen metabolism, and pancreatic insulin signalling.

Dr. Andrew Meade

Abstract

Dr. Andrew Meade will talk about the performance analysis of his Phylogeny Tree application which he ported to ACET's BladeCenter.

Bio

Andrew Meade is a Research Fellow in the School of Biological Sciences. He is the developer of a Phylogeny Tree application using Markov chains.

Dr. Amos Lawless

Approximate Gauss-Newton methods for data assimilation in environmental prediction

Variational data assimilation is a technique for retrieving the state of a system using observed data, through the minimization of a cost function constrained by a numerical model. The method is used in environmental prediction problems, for example to obtain the initial conditions for numerical weather prediction. In practice this leads to a very large nonlinear optimization problem, of several million variables, which must be solved in real-time. In order to solve this problem efficiently, operational forecasting centres apply a procedure equivalent to an approximate Gauss-Newton method. Here we examine two types of approximation used commonly in data assimilation. We establish conditions which ensure that these approximate methods converge and illustrate the results with a numerical example.

Bio

Dr Amos Lawless is a research fellow in the Mathematics Department at Reading, funded as part of the NERC-funded Data Assimilation Research Centre. His research focuses on developing the mathematical theory underpinning the practice of data assimilation. Previous to his present appointment he spent nine years working at the Met Office, developing the numerical models now used as part of their operational data assimilation system.

Prof. Mike Baines

A monitor-based moving mesh method for the solution of the compressible Euler equations

A moving mesh method is described for the numerical solution of multi-dimensional systems of conservation laws, based on the use of monitor functions. The method is derived from a conservation principle for a monitor function, interpreted as a conservation law for an artificial fluid, which generates a mesh velocity. Using a prescribed artificial vorticity, the conservation principle can be converted into an elliptic equation for a mesh velocity potential.

A distributed form of the conservation principle allows a weak form of the mesh velocity potential equation to be constructed, which is discretised using standard linear finite elements. Once the mesh velocities have been obtained the mesh is moved by an explicit time stepping routine and an Arbitrary Lagrangian Eulerian (ALE) finite volume fluid solver is used to update the solution on the moving mesh.

The method is applied to the compressible Euler equations of gas dynamics in one and two spatial dimensions. Results of the approach are shown for a number of test problems in one and two dimensions.

Bio

Prof. Mike Baines, Emeritus Professor in the Mathematics Department at the University of Reading, is an experienced numerical analyst with an international reputation in moving mesh methods and conservation laws. He has supervised many contracts and research grants, as well as numerous PhD students in applicable mathematics and MSc projects within Reading MSc course on the Numerical Solution of Differential Equations. Until recently he was Associate Editor of the Journal of Computational Physics and for many years directed the Institute for Computational Fluid Dynamics at the Universities of Oxford and Reading: under this aegis he has run Workshops and International Conferences in Computational Fluid Dynamics. He is Visiting Professor at the University of Leeds.

Prof. Simon Chandler-Wilde

Computation of Scattering by Rough Surfaces

We discuss the problem of efficiently computing acoustic or electromagnetic scattering by large rough surfaces. We briefly present algorithms based on boundary integral equation methods, with efficiency achieved via compression of the large full matrices which arise via approximation by structured matrices which reduces the asymptotic complexity in storage and computation to O(N log N) where N is the number of degrees of freedom (the size of the large matrix). Applications in optical modelling and outdoor noise propagation are briefly discussed. This is joint work with Roland Potthast and Marko Lindner (Maths), on the application side with Geoff Mitchell (Physics), and with Eric Heinemeyer (Goettingen).

Bio

Simon Chandler-Wilde is Professor of Applied Mathematics and co-leader with Vassil Alexandrov of the Computational Sciences theme at Reading. His research interests are numerical analysis and computational modelling, particularly in relation to computational acoustics and electromagnetics. Trained as a mathematician, he spent eight years as research assistant and lecturer in civil engineering, working on simulation of outdoor sound propagation problems, and this remains a research interest. More recently he has become interested in direct and inverse electromagnetic scattering. His work is currently funded by the EU, the Leverhulme Trust and by EPSRC studentships. A new project on computational modelling of optical security devices, in collaboration with Roland Potthast (Maths) and Geoff Mitchell (Physics) starts with RETF funding in January. His other activities include Chair of the Conference of Professors of Applied Mathematics, member of the Research Coordination Committee of the Institute of Acoustics, and member of the Council of the London Mathematical Society. He is co-chair for a major conference on mathematical and computational aspects of waves at Reading in July next year (Waves 2007, `www.waves2007.org`).