

CompSci07

Computational Science 2007: Interdisciplinary Challenges and Perspectives, from the Grid to e-Science

25 - 26 June 2007 at the Royal Society, London. There is no registration fee for attending this conference.

Programme

Day1: Monday, 25 June, 2007 Kohn Centre and Marble Hall booked from 9.00 A. M. to Close.

9.30 A. M. – 10.20 A. M.	Registration	
10.20 A. M. – 10.30 A. M.	Welcome and Introduction – Prof P. V. Coveney	
		Session: Setting the Context Chair: Prof B. Boghosian
10.30 A. M. - 11.00 A. M.	Prof Peter Coveney	<i>Computational Science in the Twenty-First Century</i>
11.00 A. M. - 11.30 A. M.	Prof James Annett	<i>From quantum mechanics to computational atomistic materials design: e-science challenges and opportunities from the CCP9 and Psi_k networks</i>
11.30 A. M. - 11.50 A. M.	Coffee	
		Session: Collaborative Computational Science Chair: Prof N. S. Scott
11.50 A. M. - 12.20 P. M.	Dr Helen Wright	<i>Steering and Visualization: Enabling Technologies for Computational Science</i>
12.20 P. M. - 12.40 P. M.	Prof R. S. Kalwasky	<i>Improving User Interaction in Grid based Computational Environments</i>
12.40 P. M. - 1.00 P. M.	Dr John Brooke	<i>Enabling Scientific Collaboration in Computational Science</i>
1.00 P.M. - 2.00 P. M.	Lunch	
		Session: e-Science Chair: Prof J. Annett
2.00 P. M. - 2.30 P. M.	Prof John Gurd	<i>Adaptive performance control of coupled scientific models executing in a distributed environment</i>
2.30 P. M. - 2.50 P. M.	Dr N. A. Walton	<i>Optimising the Data - Information - Knowledge Transformation: solutions for astronomy and their wider relevance</i>
2.50 P. M. - 3.20 P. M.	Prof Xavier Gonze	<i>Modern software engineering techniques applied to the simulation of materials and nanosystems : the ABINIT project</i>
3.20 P.M. - 3.35 P. M.	Coffee	
3.35 P. M. - 4.05 P. M.	Prof Wolfgang Emmerich	<i>Managing scientific workflows with BPEL</i>
4.05 P. M. - 4.25 P. M.	Dr Shantenu Jha	<i>Simple API for Grid Applications: Towards a Standardized Application Level Interface for Grids</i>
4.25 P. M. - 4.55 P. M.	Mr Stefan Zasada	<i>Production Level Scientific Simulation Management on International Federated Grids</i>
		Session: Climate Simulation Chair: Prof J. Gurd
4.55 P. M. - 5.15 P. M.	Prof Andrew Willmott	<i>Recent developments in coupled coastal and shelf sea modeling</i>
5.15 P.M. - 5.25 P. M.	Break	
		Session: Computational Biology

CompSci07

Computational Science 2007: Interdisciplinary Challenges and Perspectives, from the Grid to e-Science

25 - 26 June 2007 at the Royal Society, London. There is no registration fee for attending this conference.

		Chair: Dr H. Wright
5.25 P. M. - 5.45 P. M.	Dr Charles Laughton	<i>Challenges and Opportunities for the Development of Biomolecular Simulation</i>
5.45 P. M. - 6.05 P. M.	Prof David Gavaghan	<i>Computational Science: Implications for Education and Training</i>
6.05 P.M. - 6.15 P. M.	Break	
		Session: Physical Science Chair: Dr John Brooke
6.15 P. M. - 6.45 P. M.	Prof Sam Falle	<i>Some Computational Problems in Astrophysical Magnetohydrodynamics</i>
6.45 P. M. - 7.05 P. M.	Dr Steven Kenny	<i>Ab-initio modelling of surfaces</i>
7.05 P.M. - 7.15 P. M.	Break	
7.15 P. M. - 7.40 P. M.		Round Table Discussion

Day2: Tuesday, 26 June, 2007 Kohn Centre and Marble Hall booked from 8.30 A. M. to Close.

8.30 A. M.- 9.00 A. M.	Registration	
		Session: Grid Infrastructure in the US and UK Chair: Prof M. Cates
9.00 A. M. - 9.30 A. M	Mr Charlie Catlett	<i>TeraGrid: Analysis of Use and Impact on Science</i>
9.30 A. M. - 9.50 A. M.	Dr Stephen Pickles	<i>The National Grid Service and Computational Science</i>
9.50 A. M. - 10.10 A. M.	Mr W. T. Hewitt	<i>Overview of the NW-GRID Project - Progress to Date and Plans</i>
10.10 A. M.- 10.30 A. M.	Coffee	
		Session: Software Engineering Chair: Dr M. Nekovee
10.30 A. M. - 11.00 A. M.	Dr P. A. Couch	<i>The AgentX Framework: automating the exchange of information between scientific applications</i>
11.00 A. M. - 11.20 A. M.	Prof Ernest Laue	<i>Software development using a model driven architecture: the CCPN project</i>
11.20 A. M.- 11.25 A. M.	Break	
		Session: Computational Fluid Dynamics Chair: Prof S. Falle
11.25 A. M. - 11.55 P. M.	Prof Mike Cates	<i>Simulating Complex Fluids, Both Living and Dead</i>
11.55 P. M. - 12.15 P. M.	Dr Stewart Cant	<i>Computational Fluid Dynamics: an Engineering Perspective</i>
12.15 P. M. - 12.45 P. M.	Prof Bruce Boghosian	<i>Grid-Based Domain Decomposition for the Simulation of Hydrodynamic Turbulence</i>
12.45 P. M.- 1.45 P. M.	Lunch	
		Session: Industrial High End Computing Chair: Prof P. Durham
1.45 P. M. - 2.15 P. M.	Dr Maziar Nekovee	<i>Large-scale simulations for WiFi-based wireless telecommunication networks</i>
2.15 P. M. - 2.35 P. M.	Dr Jon Chin	<i>High Performance Computing for Interest Rate Derivatives Trading</i>
2.35 P. M. - 2.55 P. M.	Dr P. Stow	<i>The Role of High Performance Computing in CFD within Rolls Royce</i>
2.55 P. M.- 3.15 P. M.	Coffee	
		Session: e-Science and High End

CompSci07

Computational Science 2007: Interdisciplinary Challenges and Perspectives, from the Grid to e-Science

25 - 26 June 2007 at the Royal Society, London. There is no registration fee for attending this conference.

		Computing Chair: Prof P. V. Coveney
3.15 P. M. - 3.45 P. M.	Dr T. Schulthess	<i>Software Interoperability in Computational Nano- and Materials Science</i>
3.45 P. M. - 4.05 P. M.	Prof M. Atkinson	<i>Software Services for Science from e-Science: the emergence of software as a facility</i>
4.05 P. M. - 4.30 P. M.		Round Table Discussion