

University of Nottingham High Performance Computing Conference 2008

Small Lecture Theatre, School of Chemistry, University of Nottingham

PROGRAMME

Tuesday 8th January

9:30 REGISTRATION (Chemistry Building, Foyer)

10:25 Jonathan Hirst Welcome from Chair
10:30 Chris Booth *hpc@nottingham - the old and the new*
11:00 Mark Greenaway *Applications of HPC in THz electronics*
11:30 Mark Oakley *Simulations of Supercritical Fluids*
12:00 Jaume Bacardit *Data Mining Large-scale Bioinformatics Datasets*

12:30 LUNCH & POSTERS

Frazer Pearce (Chair)

14:00 Kim Evans *Comparing protein surfaces for similar binding sites*
14:30 Will Hartley *Distant galaxies: ever increasing numbers*
15:00 Stephen Hamby *High throughput computing and protein structure*

15:30 TEA

Carol Eastwick (Chair)

16:00 Keith Benedict *Bose Condensates - Mean Field Dynamics and Beyond*
16:30 James Smaldon *Membrane Simulations with a Parallel Implementation of Dissipative Particle Dynamics*
17:00 Michael Lees *Meshless numerical methods and GPU computing*

Wednesday 9th January

Phil Williams (Chair)

10:30 Liz Bailes *Origins of Human AIDS Viruses*
11:00 Mike Stout *Predicting Aspects of Protein Structure Using Evolutionary Computation*
11:30 Michael Mazanetz *Exploiting Protein Flexibility in Molecular Recognition*
12:00 Bissan Al-Lazikani (Discovery Informatics, BioFocus DPI) *Knowledge-based approaches to solving drug discovery problems*

13:00 LUNCH & POSTERS

Chris Booth (Chair)

14:30 Lorena Gazzola *Simulating the Universe: gas physics in the millennium run*
15:00 David Robinson *Fluorescence calculations using high level ab initio techniques*
15:30 Technology update – Chris Roberts (HP) / Tim Cooke (Streamline)

16:30 DRINKS & CLOSE