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Crossing boundaries: computational science, e-Science and global e-Infrastructure - volumes I and II

Compiled and edited by Peter Coveney and Malcolm P Atkinson

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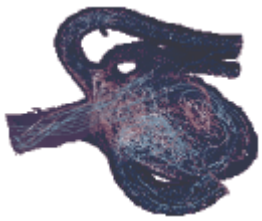

Crossing boundaries: computational science, e-Science and global e-Infrastructure I and II contain a selection of papers presented at the UK e-Science All Hands conference, held in Edinburgh between the 8 and 11 September 2008 (http://www.allhands.org.uk/archive/2008/).

The conference aimed to bring together computer scientists, computational scientists and researchers from all domains engaged in the endeavour of e-Science: computationally intensive research, typically carried out in highly distributed environments (often involving grid computing), with potentially immense data sets, involving technologies/resources that enable and facilitate such distributed collaboration.

Fewer than 15% of the papers submitted to the conference made it through the rigorous review process to publication in these two issues. The papers selected for publication can be considered to represent the cutting edge of e-Science, paving the way towards a new, faster, better and different science than has been possible before. The full contents of both volumes are detailed below and overleaf.

Crossing boundaries: computational science, e-Science and global e-Infrastructure I and II comprise issues 1897 and 1898 of *Philosophical Transactions A: Mathematical, Physical and Engineering Sciences* and the full content of both issues can be accessed at **http://rsta.royalsocietypublishing.org/site/issues/computational_eScience.xhtml**

The print issues can be purchased at the discounted price shown above. To place an order at this price, please visit the above URL and, when prompted, enter **TA 1897 for Vol 1** and/or **TA 1898 for Vol 2**.

Volume I

Introduction: Crossing boundaries: computational science, e-Science and global e-Infrastructure – PV Coveney and MP Atkinson

Sector and Sphere: the design and implementation of a high-performance data cloud – Y Gu and RL Grossman

GridPP: the UK grid for particle physics – D Britton, AJ Cass, PEL Clarke, J Coles, DJ Colling, AT Doyle, NI Geddes, JC Gordon, RWL Jones, DP Kelsey, SL Lloyd, RP Middleton, GN Patrick, RA Sansum and SE Pearce

Louisiana: a model for advancing regional e-Research through cyberinfrastructure – DS Katz, G Allen, R Cortez, C Cruz-Neira, R Gottumukkala, ZD Greenwood, L Guice, S Jha, R Kolluru, T Kosar, L Leger, H Liu, C McMahon, J Nabrzyski, B Rodriguez-Milla, E Seidel, G Speyrer, M Stubblefield, B Voss and S Whittenburg

Building a scientific data grid with DIGS – MG Beckett, CR Allton, CTH Davies, I Davis, JM Flynn, EJ Grant, RS Hamilton, AC Irving, RD Kenway, RH Ostrowski, JT Perry, JR Swedlow and A Trew

Flexible selection of heterogeneous and unreliable services in large-scale grids – S Stein, TR Payne and NR Jennings

Standards-based network monitoring for the grid – J Nowell, K Kavoussanakis, C Palansuriya, M Piotrowski, F Scharinger, P Graham, B Dobrzelecki and A Trew

The Archaeotools project: faceted classification and natural language processing in an archaeological context – S Jeffrey, J Richards, F Ciravegna, S Waller, S Chapman and Z Zhang

Integrating Open Grid Services Architecture Data Access and Integration with computational Grid workflows – T Kukla, T Kiss, P Kacsuk and G Terstyanszky

Improved performance control on the Grid – ME Tellier, GD Riley and TL Freeman

Novel submission modes for tightly coupled jobs across distributed resources for reduced time-to-solution – P Chakraborty, S Jha and DS Katz

Real science at the petascale – RS Saksena, B Boghosian, L Fazendeiro, OA Kenway, S Manos, MD Mazzeo, SK Sadiq, JL Suter, D Wright and PV Coveney

Enabling cutting-edge semiconductor simulation through grid technology – D Reid, C Millar, S Roy, G Roy, R Sinnott, G Stewart, G Stewart and A Asenov

UKQCD software for lattice quantum chromodynamics – PA Boyle, RD Kenway and CM Maynard

Adaptive distributed replica—exchange simulations – A Luckow, S Jha, J Kim, A Merzky and B Schnor

High-performance computing for Monte Carlo radiotherapy calculations – P Downes, G Yaikhom, JP Giddy, DW Walker, E Spezi and DG Lewis

Volume II

Preface: Crossing boundaries: computational science, e-Science and global e-Infrastructure – PV Coveney and MP Atkinson

Multi-objective optimization of GENIE Earth system models – AR Price, RJ Myerscough, II Voutchkov, R Marsh and SJ Cox

Bringing simulation to engineers in the field: a Web 2.0 approach – R Haines, K Khan and J Brooke

The OptIPuter microscopy demonstrator: enabling science through a transatlantic lightpath – M Ellisman, T Hutton, A Kirkland, A Lin, C Lin, T Molina, S Peltier, R Singh, K Tang, AE Trefethen, DCH Wallom and X Xiong

Adaptation and development of software simulation methodologies for cardiovascular engineering: present and future challenges from an end-user perspective – V Díaz-Zuccarini, AJ Narracott, G Burriesci, C Zervides, D Rafiroiu, D Jones, DR Hose and PV Lawford

Using high-resolution displays for high-resolution cardiac data – C Goodyer, J Hodrien, J Wood, P Kohl and K Brodlie

Federating distributed clinical data for the prediction of adverse hypotensive events – A Stell, R Sinnott, J Jiang, R Donald, I Chambers, G Citerio, P Enblad, B Gregson, T Howells, K Kiening, P Nilsson, A Ragauskas, J Sahuquillo and I Piper

HIV decision support: from molecule to man – PMA Sloot, PV Coveney, G Ertaylan, V Müller, CA Boucher and M Bubak

A computational Grid framework for immunological applications – MD Halling-Brown, DS Moss, CE Sansom and AJ Shepherd

Information security: where computer science, economics and psychology meet – R Anderson and T Moore

Data protection in grid-based multicentric clinical trials: killjoy or confidence-building measure? – M Arning, N Forgó and T Krügel

Engineering design optimization using services and workflows – T Crick, P Dunning, H Kim and J Padget

A user-orientated approach to provenance capture and representation for *in silico* experiments, explored within the atmospheric chemistry community – CJ Martin, MH Haji, PK Jimack, MJ Pilling and PM Dew

AMUC: Associated Motion capture User Categories – SJ Norman, SEM Lawson, P Olivier, P Watson, AM-A Chan, M Dade-Robertson, P Dunphy, D Green, H Hiden, J Hook and DG Jackson

MoSeS: Modelling and Simulation for e-Social Science – P Townend, J Xu, M Birkin, A Turner and B Wu

Dancing on the Grid: using e-Science tools to extend choreographic research – H Bailey, M Bachler, SB Shum, A Le Blanc, S Popat, A Rowley and M Turner