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Computational Science – ICCS 2006

6th International Conference
Reading, UK, May 28-31, 2006
Proceedings, Part I

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Library of Congress Control Number: 2006926429

CR Subject Classification (1998): F, D, G, H, I, J, C.2-3

LNCS Sublibrary: SL 1 – Theoretical Computer Science and General Issues

ISSN	0302-9743
ISBN-10	3-540-34379-2 Springer Berlin Heidelberg New York
ISBN-13	978-3-540-34379-0 Springer Berlin Heidelberg New York

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springer.com

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Printed in Germany

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, India
Printed on acid-free paper SPIN: 11758501 06/3142 5 4 3 2 1 0

Preface

The Sixth International Conference on Computational Science (ICCS 2006) was held in Reading, United Kingdom, May 28-31 and continued the traditions of previous conferences in the series: ICCS 2005 in Atlanta, Georgia, USA; ICCS 2004 in Krakow, Poland; ICCS 2003 held simultaneously at two locations in, Melbourne, Australia and St. Petersburg, Russia; ICCS 2002 in Amsterdam, The Netherlands; and ICCS 2001 in San Francisco, California, USA.

Since the first conference in San Francisco, rapid developments in Computational Science as a mainstream area facilitating multi-disciplinary research essential for the advancement of science have been observed. The theme of ICCS 2006 was “Advancing Science through Computation”, marking several decades of progress in Computational Science theory and practice, leading to greatly improved applications science. The conference focused on the following major themes: tackling Grand Challenges Problems; modelling and simulations of complex systems; scalable algorithms and tools and environments for Computational Science. Of particular interest were the following major recent developments in novel methods and modelling of complex systems for diverse areas of science, scalable scientific algorithms, advanced software tools, computational grids, advanced numerical methods, and novel application areas where the above novel models, algorithms and tools can be efficiently applied such as physical systems, computational and systems biology, environmental systems, finance, and others.

Keynote lectures were delivered by Mateo Valero (Director, Barcelona Supercomputing Centre) - “Tackling Grand Challenges Problems”; Chris Johnson (Distinguished Professor, University of Utah) - “Visualizing the Future”; José Moreira (IBM, Chief Architect, Commercial Scale Out) - “Achieving Breakthrough Science with the Blue Gene/L Supercomputer”; Martin Curley (INTEL, Global Director of Innovation and IT Research) - “IT Innovation: A New Era”; Vaidy Sunderam (Samuel Candler Dobbs Professor of Computer Science, Emory University, USA) - “Metacomputing Revisited: Alternative Paradigms for Distributed Resource Sharing”; and Ron Bell (AWE plc.) - “The AWE HPC Benchmark”.

In addition, two special sessions were held - one by industry and one by the funding bodies. Three tutorials preceded the main technical program of the conference: “Tools for Program Analysis in Computational Science” by Dieter Kranzlmüller; “P-GRADE Portal” by P. Kascuk, T. Kiss and G. Sipos; and “Scientific Computing on Graphics Hardware” by Dominik Göddeke. We would like to thank all the keynote, the invited, and the tutorial speakers for their inspiring talks.

Apart from the plenary sessions and tutorials the conference included twelve parallel oral sessions and two poster sessions. Since the first ICCS in San

Francisco the conference has grown steadily attracting increasing numbers of researchers in the field of Computational Science. For ICCS 2006 we received over 1,400 submissions, around 300 for the main track and over 1,100 for the originally proposed workshops. Of these submissions, 98 were accepted as full papers and 29 as posters for the main track; and 500 were accepted as full papers, short papers or posters for the 32 workshops. This selection was possible due to the tremendous work done by the Program Committee and the 720 reviewers. The author index contains over 1,000 names and over 600 participants from all the major continents. The papers cover a wide variety of topics in Computational Science, ranging from Grand Challenges problems and modelling of complex systems in various areas to advanced numerical algorithms and new scalable algorithms in diverse application areas and software environments for Computational Science. The ICCS 2006 Proceedings consist of four volumes, 3991 to 3994, where the first volume contains the papers from the main track and all the posters; the remaining three volumes contain the papers from the workshops. ICCS this year is primarily published on a CD and we would like to thank Springer for their cooperation and partnership. We hope that the ICCS 2006 Proceedings will be a major intellectual resource for many computational scientists and researchers for years ahead. During the conference the best papers from the main track and workshops as well as the best posters were nominated and commended on ICCS 2006 website. A number of selected papers will also be published in special issues of relevant mainstream journals.

We would like to thank all workshop organisers and the program committee for the excellent work, which further enhanced the conference's standing and led to very high quality event with excellent papers. We would like to express our gratitude to Advanced Computing and Emerging Technologies Centre staff, postgraduates and students for their wholehearted support of ICCS 2006. We would like to thank the School of Systems Engineering, Conference Office, Finance Department and various units at the University of Reading for different aspects of the organization and for their constant support in making ICCS 2006 a success. We would like to thank the Local Organizing Committee for their persistent and enthusiastic work towards the success of ICCS 2006. We owe special thanks to our sponsors: Intel, IBM, SGI, Microsoft Research, EPSRC and Springer; and to ACET Centre and the University of Reading for their generous support. We would like to thank SIAM, IMACS, and UK e-Science programme for endorsing ICCS 2006.

ICCS 2006 was organized by the Advanced Computing and Emerging Technologies Centre, University of Reading, with support from the Section Computational Science at the Universiteit van Amsterdam and Innovative Computing Laboratory at the University of Tennessee, in cooperation with the Society for Industrial and Applied Mathematics (SIAM), the International Association for Mathematics and Computers in Simulation (IMACS), and the UK Engineering and Physical Sciences Research Council (EPSRC). We invite you to visit the ICCS 2006 website (<http://www.iccs-meeting.org/iccs2006/>) and ACET Centre website (<http://www.acet.reading.ac.uk/>) to recount the events leading up

to the conference, to view the technical programme, and to recall memories of three and a half days of engagement in the interest of fostering and advancing Computational Science.

June 2006

Vassil N. Alexandrov
G. Dick van Albada
Peter M.A. Sloot
Jack J. Dongarra

Organisation

ICCS 2006 was organised by the Centre for Advanced Computing and Emerging Technologies (ACET), University of Reading, UK, in cooperation with the University of Reading (UK), the Universiteit van Amsterdam (The Netherlands), the University of Tennessee (USA), Society for Industrial and Applied Mathematics (SIAM), International Association for Mathematics and Computers in Simulation (IMACS) and Engineering and Physical Sciences Research Council (EPSRC). The conference took place on the Whiteknights Campus of the University of Reading.

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Tools for Program Development and Analysis in Computational Science

D. Kranzlmüller - GUP, Joh. Kepler University, Linz, Austria
R. Wismüller - University of Siegen, Germany
A. Bode - Technische Universität München, Germany
J. Volkert - GUP, Joh. Kepler University, Linz, Austria

Collaborative and Cooperative Environments

C. Anthes - GUP, Joh. Kepler University, Linz, Austria
V.N. Alexandrov - ACET, University of Reading, UK
D.J. Roberts - NICVE, University of Salford, UK
J. Volkert - GUP, Joh. Kepler University, Linz, Austria
D. Kranzlmüller - GUP, Joh. Kepler University, Linz, Austria

Second International Workshop on Bioinformatics Research and Applications (IWBRA'06)

A. Zelikovsky - Georgia State University, USA
Y. Pan - Georgia State University, USA
I.I. Mandoiu - University of Connecticut, USA

Third International Workshop on Practical Aspects of High-Level Parallel Programming (PAPP 2006)

A. Benoît - Laboratoire d'Informatique du Parallélisme, Ecole Normale Supérieure de Lyon, France
F. Loulergue - LIFO, Université d'Orléans, France

Wireless and Mobile Systems

H. Choo - Networking Laboratory, Sungkyunkwan University, Suwon, KOREA

GeoComputation

Y. Xue - Department of Computing, Communications Technology and Mathematics, London Metropolitan University, UK

Computational Chemistry and Its Applications

P. Ramasami - Department of Chemistry, University of Mauritius

Knowledge and Information Management in Computer Communication Systems (KIMCCS 2006)

N.T. Nguyen - Institute of Control and Systems Engineering,
Wroclaw University of Technology, Poland

- A. Grzech - Institute of Information Science and Engineering,
Wroclaw University of Technology, Poland
R. Katarzyniak - Institute of Information Science and Engineering,
Wroclaw University of Technology, Poland

Modelling of Complex Systems by Cellular Automata (MCSCA 2006)

- J. Kroc - University of West Bohemia, Czech Republic
T. Suzudo - Japan Atomic Energy Agency, Japan
S. Bandini - University of Milano - Bicocca, Italy

Dynamic Data Driven Application Systems (DDDAS 2006)

- F. Darema - National Science Foundation, USA

Parallel Monte Carlo Algorithms for Diverse Applications in a Distributed Setting

- I.T. Dimov - ACET, University of Reading, UK
V.N. Alexandrov - ACET, University of Reading, UK

International Workshop on Intelligent Storage Technology (IST06)

- J. Shu - Department of Computer Science and Technology, Tsinghua University,
Beijing, P.R. China

Intelligent Agents in Computing Systems

- R. Schaefer - Department of Computer Science, Stanislaw Staszic University
of Science and Technology in Kraków
K. Cetnarowicz - Department of Computer Science, Stanislaw Staszic University
of Science and Technology in Kraków

First International Workshop on Workflow Systems in e-Science (WSES06)

- Z. Zhao - Informatics Institute, University of Amsterdam, The Netherlands
A. Belloum - University of Amsterdam, The Netherlands

Networks: Structure and Dynamics

- B. Tadic - Theoretical Physics Department, J. Stefan Institute, Ljubljana,
Slovenia
S. Thurner - Complex Systems Research Group, Medical University Vienna,
Austria

Evolution Toward Next Generation Internet (ENGI)

Y. Cui - Tsinghua University, P.R. China

T. Korkmaz - University of Texas at San Antonio, USA

**General Purpose Computation on Graphics Hardware (GPGPU):
Methods, Algorithms and Applications**

D. Göldeke - Universität Dortmund, Institut für Angewandte Mathematik
und Numerik, Germany

S. Turek - Universität Dortmund, Institut für Angewandte Mathematik
und Numerik, Germany

Intelligent and Collaborative System Integration Technology (ICSIT)

J.-W. Lee - Center for Advanced e-System Integration Technology,
Konkuk University, Seoul, Korea

Computational Methods for Financial Markets

R. Simutis - Department of Informatics, Kaunas Faculty, Vilnius University,
Lithuania

V. Sakalauskas - Department of Informatics, Kaunas Faculty, Vilnius University,
Lithuania

D. Kriksčiuniene - Department of Informatics, Kaunas Faculty,
Vilnius University, Lithuania

**2006 International Workshop on P2P for High Performance
Computational Sciences (P2P-HPCS06)**

H. Jin - School of Computer Science and Technology, Huazhong University of
Science and Technology, Wuhan, China

X. Liao - Huazhong University of Science and Technology, Wuhan, China

Computational Finance and Business Intelligence

Y. Shi - Graduate School of the Chinese Academy of Sciences, Beijing, China

**Third International Workshop on Automatic Differentiation Tools
and Applications**

C. Bischof - Inst. for Scientific Computing, RWTH Aachen University, Germany

S.A. Forth - Engineering Systems Department, Cranfield University,
RMCS Shrivenham, UK

U. Naumann - Software and Tools for Computational Engineering,
RWTH Aachen University, Germany

J. Utke - Mathematics and Computer Science Division, Argonne National
Laboratory, IL, USA

2006 Workshop on Scientific Computing in Electronics Engineering

Y. Li - National Chiao Tung University, Hsinchu City, Taiwan

New Trends in the Numerical Solution of Structured Systems with Applications

T. Politi - Dipartimento di Matematica, Politecnico di Bari, Itali

L. Lopez - Dipartimento di Matematica, Università di Bari, Itali

Workshop on Computational Science in Software Engineering (CSSE'06)

D. Rodríguez García - University of Reading, UK

J.J. Cuadrado - University of Alcalá, Spain

M.A. Sicilia - University of Alcalá, Spain

M. Ruiz - University of Cádiz, Spain

Digital Human Modeling (DHM-06)

Y. Cai - Carnegie Mellon University, USA

C. Imielinska - Columbia University

Real Time Systems and Adaptive Applications (RTSAA 06)

T. Kuo - National Taiwan University, Taiwan

J. Hong - School of Computer Science and Engineering, Kwangwoon University, Seoul, Korea

G. Jeon - Korea Polytechnic University, Korea

International Workshop on Grid Computing Security and Resource Management (GSRM'06)

J.H. Abawajy - School of Information Technology, Deakin University, Geelong, Australia

Fourth International Workshop on Autonomic Distributed Data and Storage Systems Management Workshop (ADSM 2006)

J.H. Abawajy - School of Information Technology, Deakin University, Geelong, Australia

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