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2013 International Conference on Computational Science

# Computation at the Frontiers of Science, preface for ICCS 2013

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Welcome to the 13<sup>th</sup> Annual International conference on Computational Science, to be held 5th-7th June 2013 in Barcelona, Spain. This year's conference will take place in the beautiful city of Barcelona at CCIB Congress center on the beach. ICCS 2013 is organized by the Barcelona Super Computing Centre, Universiteit van Amsterdam, the University of Tennessee and Nanyang Technological University.

The International Conference on Computational Science is an annual conference that brings together researchers and scientists from mathematics and computer science as basic computing disciplines, researchers from various application areas who are pioneering computational methods in sciences such as physics, chemistry, life sciences, and engineering, as well as in arts and humanitarian fields, to discuss problems and solutions in the area, to identify new issues, and to shape future directions for research.

Since its inception in 2001, ICCS has attracted increasingly higher quality and numbers of attendees and papers and this year is not an exception. This year we expect over 350 participants. The proceedings series have become a major intellectual resource for computational science researchers and serve to both define and advance the state of the art of the field.

ICCS 2013 in Barcelona will be the thirteenth in this series of highly successful conferences. For the previous twelve meetings see: http://www.iccs-meeting.org/iccs2013/previous-iccs.html

The theme for ICCS 2013 is "Computation at the Frontiers of Science", to mark the ever-increasing importance of and progress in computational science theory and practice at the frontiers of science. The conference will be a unique event focusing on recent developments in computational methods for modelling complex systems in diverse areas of science, scalable scientific algorithms, advanced software tools, computational grids, advanced numerical methods. ICCS2013 will also feature the important advances in computational science towards exascale computing. ICCS includes work focusing on the application of these methods in diverse areas including, Computational Biology, Computational Finance, Earth Sciences, Social Sciences and more.

For this great event, World leading keynote speakers were invited, to give their current and future vision of Computational Science.

- Hesham Ali, University of Nebraska, Omaha, USA
- Steve Furber, University of Manchester, UK
- Thierry van der Pyl, DG CONNECT, European Commission
- David De Roure, Oxford e-Research Centre, UK
- Vladimir Voevodin, Moscow State University, Russia
- Raimond Winslow, The Johns Hopkins University, Baltimore MD, USA

Besides our excellent keynote speakers, out of the submitted papers to main track and workshops, we selected over 300 high-quality papers for presentation at the conference and publication in the proceedings, published by Elsevier in their Procedia Computer Science series.

ICCS relies strongly on the vital contributions of our workshop organizers to attract high quality papers in many subject areas. We would like to thank all committee members for the main track and the workshops for their contribution to ensure a high standard for the accepted papers. We would also like to say a special thanks to the people who ensured all papers adhered to the correct formatting for publication. Finally the committee would like to thank Prof. Dick van Albada, whose continuing support for the conference has been essential to its success.

We are proud to note that ICCS is an ERA 2010 A-ranked conference series.

We wish you a successful and enjoyable conference in Barcelona.

June 2013,

The ICCS 2013 Organizers,
Vassil Alexandrov
Michael Lees
Valeria Krzhizhanovskaya
Jack Dongarra
Peter M.A. Sloot

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### Workshops and Organizers

### 7th Workshop on Computational Chemistry and Its Applications

Ponnadurai Ramasami, University of Mauritius, Mauritius

### 4th Workshop on Computational Optimization, Modelling and Simulation (COMS 2013)

X.S. Yang, National Physical Lab, UK; S. Koziel, Rekjavik University, Iceland; L. Leifsson, Rekjavik University, Iceland

#### 10th International Workshop on Modeling and Computing Multiscale Systems

Valeria Krzhizhanovskaya and Alfons Hoekstra University of Amsterdam, The Netherlands; Katarzyna Rycerz, Institute of Computer Science and CYFRONET, AGH, Krakow, Poland; Derek Groen, University College London, UK; Eric Lorenz, University of Amsterdam, The Netherlands; Bartosz Bosak, PSNC, Poznan, Poland

### Workshop on Computational and Algorithmic Finance

Andrey Itkin, Numerix LLC and New York University

### Knowledge representation and applied models and metadata in computational science

Miguel-Angel Sicilia, Computer Science Department, University of Alcalá, Spain; Nikos Manouselis, Agro-Know Technologies, Greece; Pythagoras Karampiperis, National Center of Scientific Research, Demokritos

# 3rd International Workshop on Advances in High-Performance Computational Earth Sciences: Applications & Frameworks

Yifeng CuiSan Diego Supercomputer Center, USA; Xing Cai Simula Research Laboratory, Norway

### Eighth international Workshop on Automatic Performance Tuning (iWAPT2013)

Takeshi Iwashita, Kyoto University, Japan; Franz Franchetti, Carnegie Mellon University, USA

### 6th Workshop on Biomedical and Bioinformatics Challenges for Computer Science (BBC 2013)

Mario Cannataro, University Magna Gri¿½cia of Catanzaro, Italy; Werner Dubitzky, University of Ulster, United Kingdom; Joakim Sundnes, Simula Research Laboratory, Norway; Rodrigo Weber dos Santos, Federal University of Juiz de Fora, Brazil

### 7th Workshop on Teaching Computational Science (WTCS 2012)

A.B. Shiflet, Wofford College, USA; A. Tirado-Ramos, Emory University, USA

### Agent-Based Simulations, Adaptive Algorithms and Solvers

Robert Schaefer, Krzysztof Cetnarowicz, Maciej Paszynski, AGH University of Science and Technology, Poland; Victor Calo, King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia; David Pardo, UPV/EHU, Spain; Emilio Luque, Universitat Autonoma de Barcelona, Spain

# Architecture, Languages, Compilation and Hardware support for Emerging ManYcore systems (ALCHEMY 2013)

Loïc Cudennec, and Stéphane Louise, CEA LIST, France

### 10th Workshop on Computational Finance and Business Intelligence

Y. Shi, Graduate University of the Chinese Academy of Sciences and University of Nebraska at Omaha; S.Y. Wang, Academy of Mathematical and System Sciences, Chinese Academy of Sciences; Y. Tian, Graduate University of the Chinese Academy of Sciences

### Tools for Program Development and Analysis in Computational Science

Karl Fürlinger, D. Kranzlmüller, Ludwig-Maximilians-Universität München, Germany; Arndt Bode, TUM, Germany; A. Knüpfer, Universität Dresden; J. Tao, Karlsruhe Institute of Technology; Jens Volkert, JKU, Austria; R. Wismüller, University of Siegen;

# Second Workshop on Educational Approaches for Integrating Bioinformatics into Computer and Life Science

Mark A. Pauley and William E. Tapprich, University of Nebraska at Omaha, USA

### **Dynamic Data Driven Application Systems - DDDAS 2012**

C.C. Douglas, University of Wyoming, USA; A. Patra, University of Buffalo, USA; Ana Cortés, Universitat Autonoma de Barcelona, Spain

### 2<sup>nd</sup> Workshop on Computational Approaches to Social Modeling (ChASM)

Bruno Gonçalves, Nicola Perra, A. Baronchelli, Notheastern University, USA

### International Workshop on Computational Flow and Transport: Modeling, Simulations and Algorithms

S. Sun, King Abdullah University of Science and Technology; J Liu, Colorado State University, USA

### **Urgent Computing: Computations for Decision Support in Critical Situations**

Anna Bilyatdinova, Anna Kalyuzhnaya and Sergey Ivanov, Saint-Petersburg National Research University of Information Technologies, Mechanics and Optics, Russia

### **Large Scale Computational Physics**

E.H.J. de Doncker, Western Michigan University and Fukuko Yuasa, High Energy Accelerator Research Organization, Japan

### **Solving Problems with Uncertainties**

Vassil Alexandrov, ICREA-Barcelona Supercomputing Centre, Spain

### 4th Workshop on Data Mining in Earth System Science (DMESS 2013)

F.M. Hoffman, J Kumar, J.W Larson, Oak Ridge National Laboratory and ANL, USA; M.D. Mahecha, Max Planck Institute for Biogeochemistry

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