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Computational Science – ICCS 2005

5th International Conference
Atlanta, GA, USA, May 22-25, 2005
Proceedings, Part I



Springer

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Preface

The Fifth International Conference on Computational Science (ICCS 2005) held in Atlanta, Georgia, USA, May 22–25, 2005, continued in the tradition of previous conferences in the series: 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.

Computational science is rapidly maturing as a mainstream discipline. It is central to an ever-expanding variety of fields in which computational methods and tools enable new discoveries with greater accuracy and speed. ICCS 2005 was organized as a forum for scientists from the core disciplines of computational science and numerous application areas to discuss and exchange ideas, results, and future directions. ICCS participants included researchers from many application domains, including those interested in advanced computational methods for physics, chemistry, life sciences, engineering, economics and finance, arts and humanities, as well as computer system vendors and software developers. The primary objectives of this conference were to discuss problems and solutions in all areas, to identify new issues, to shape future directions of research, and to help users apply various advanced computational techniques. The event highlighted recent developments in algorithms, computational kernels, next generation computing systems, tools, advanced numerical methods, data-driven systems, and emerging application fields, such as complex systems, finance, bioinformatics, computational aspects of wireless and mobile networks, graphics, and hybrid computation. Keynote lectures were delivered by John Drake – High End Simulation of the Climate and Development of Earth System Models; Marian Bubak – Towards Knowledge – Based Computing: Personal Views on Recent Developments in Computational Science and the CrossGrid Project; Alok Choudhary – Large Scale Scientific Data Management; and David Keyes – Large Scale Scientific Discovery through Advanced Computing.

In addition, four invited presentations were delivered by representatives of industry: David Barkai from Intel Corporation, Mladen Karcic from IBM, Steve Modica from SGI and Dan Fay from Microsoft. Seven tutorials preceded the main technical program of the conference: Tools for Program Analysis in Computational Science by Dieter Kranzlmüller and Andreas Knüpfer; Computer Graphics and Geometric Modeling by Andrés Iglesias; Component Software for High Performance Computing Using the CCA by David Bernholdt; Computational Domains for Explorations in Nanoscience and Technology, by Jun Ni, Deepak Srivastava, Shaoping Xiao and M. Meyyappan; Wireless and Mobile Communications by Tae-Jin Lee and Hyunseung Choo; Biomedical Literature Mining and Its Applications in Bioinformatics by Tony Hu; and Alternative Approaches to

Grids and Metacomputing by Gunther Stuer. We would like to thank all keynote, invited and tutorial speakers for their interesting and inspiring talks.

Aside from the plenary lectures, the conference included 10 parallel oral sessions and 3 poster sessions. Ever since the first meeting in San Francisco, ICCS has attracted an increasing number of researchers involved in the challenging field of computational science. For ICCS 2005, we received 464 contributions for the main track and over 370 contributions for 24 originally-proposed workshops. Of these submissions, 134 were accepted as full papers accompanied by oral presentations, and 89 for posters in the main track, while 241 papers were accepted for presentations at 21 workshops. This selection was possible thanks to the hard work of the 88-member Program Committee and 362 reviewers. The author index contains 1395 names, and over 500 participants from 41 countries and all continents attended the conference. The ICCS 2005 proceedings consists of three volumes. The first volume, LNCS 3514, contains the full papers from the main track of the conference, while volumes 3515 and 3516 contain the papers accepted for the workshops and short papers. The papers cover a wide range of topics in computational science, ranging from numerical methods, algorithms, and computational kernels to programming environments, grids, networking and tools. These contributions, which address foundational and computer science aspects are complemented by papers discussing computational applications in a variety of domains. ICCS continues its tradition of printed proceedings, augmented by CD-ROM versions for the conference participants. We would like to thank Springer for their cooperation and partnership. We hope that the ICCS 2005 proceedings will serve as a major intellectual resource for computational science researchers for many years to come. During the conference the best papers from the main track and workshops as well as the best posters were nominated and commended on the ICCS 2005 Website. A number of papers will also be published in special issues of selected journals.

We owe thanks to all workshop organizers and members of the Program Committee for their diligent work, which led to the very high quality of the event. We would like to express our gratitude to Emory University and Emory College in general, and the Department of Mathematics and Computer Science in particular, for their wholehearted support of ICCS 2005. We are indebted to all the members of the Local Organizing Committee for their enthusiastic work towards the success of ICCS 2005, and to numerous colleagues from various Emory University units for their help in different aspects of organization. We very much appreciate the help of Emory University students during the conference. We owe special thanks to our corporate sponsors: Intel, IBM, Microsoft Research, SGI, and Springer; and to ICIS, Math & Computer Science, Emory College, the Provost's Office, and the Graduate School at Emory University for their generous support. ICCS 2005 was organized by the Distributed Computing Laboratory at the Department of Mathematics and Computer Science at Emory University, with support from the Innovative Computing Laboratory at the University of Tennessee and the Computational Science Section at the University of Amsterdam, in cooperation with the Society for Industrial and Applied Mathe-

matics (SIAM). We invite you to visit the ICCS 2005 Website (<http://www.iccs-meeting.org/ICCS2005/>) to recount the events leading up to the conference, to view the technical program, and to recall memories of three and a half days of engagement in the interest of fostering and advancing computational science.

June 2005

Vaidy Sunderam
on behalf of
G. Dick van Albada,
Jack J. Dongarra,
Peter M.A. Sloot

Organization

ICCS 2005 was organized by the Distributed Computing Laboratory, Department of Mathematics and Computer Science, Emory University, Atlanta, GA, USA, in cooperation with Emory College, Emory University (USA), the University of Tennessee (USA), the University of Amsterdam (The Netherlands), and the Society for Industrial and Applied Mathematics (SIAM). The conference took place on the campus of Emory University, in Atlanta, Georgia, USA.

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