International Conference on Computational Science, ICCS 2017, 12-14 June 2017,
Zurich, Switzerland

The Art of Computational Science,
Bridging Gaps – Forming Alloys.
Preface for ICCS 2017

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Introduction

Welcome to the 17th Annual International Conference on Computational Science (ICCS -
http://www.iccs-meeting.org), to be held on June 12-14, 2017 in Zürich, Switzerland. Located in
central Europe close to the Alps, Zürich is Switzerland’s largest city and one of the world’s main
financial hubs. In addition to the Swiss Federal Institute of Technology (or “Eidgenössische
Technische Hochschule Zürich” (ETH) in German), one of the world’s most distinguished research
institutions and the proud host of ICCS 2017, Zürich is home to many parks, museums and churches.
The city stretches out on both sides of the Limmat river, which flows out of the beautiful Lake Zürich.
ICCS 2017 is organized by ETH Zürich, University of Amsterdam, NTU Singapore and the University
of Tennessee.

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, with over 300 expected participants. The
proceedings series have become a major intellectual resource for computational science researchers,
defining and advancing the state of the art in this field.

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ICCS 2017 in Zürich, Switzerland, will be the seventeenth in this series of highly successful conferences. For the previous sixteen meetings see: http://www.iccs-meeting.org/iccs2017/previous-iccs/

The theme for ICCS 2017 is "The Art of Computational Science. Bridging Gaps – Forming Alloys", to highlight the role of computation as a fundamental method of scientific inquiry and technological discovery tackling problems across scientific domains and creating synergies between disciplines. This conference will be a unique event focusing on recent developments in: scalable scientific algorithms; advanced software tools; computational grids; advanced numerical methods; and novel application areas. These innovative novel models, algorithms and tools drive new science through efficient application in areas such as physical systems, computational and systems biology, environmental systems, finance, and others.

ICCS is well known for its excellent line up of keynote speakers. The keynotes for 2017 are:

- Anastasia Ailamaki, École Polytechnique Fédérale de Lausanne, Switzerland
- Efthimios Kaxiras, Harvard University, USA
- Michael Norman, San Diego Supercomputer Center, UC San Diego, USA
- Tomaso Poggio, Eugene McDermott Professor, MIT, USA
- Olga Sorkine-Hornung, ETH Zürich, Switzerland
- Rick L. Stevens, Argonne National Laboratory, USA
- Stefan Thurner, Medical University of Vienna, Austria

This year we had 625 submissions (267 submissions to the main track and 358 to the workshops). In the main track, 74 full papers were accepted (28%). In the workshops, 151 full papers (42%). A high acceptance rate in the workshops is explained by the nature of these thematic sessions, where many experts in a particular field are personally invited by workshop organisers to participate in their sessions.

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 workshops for their contribution to ensure a high standard for the accepted papers. We would also like to thank Elsevier and Intellegibilis for their support.

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

We wish you a successful and enjoyable conference in Zürich.

June 2017

The ICCS 2017 Organizers:
- Petros Koumoutsakos
- Eleni Chatzi
- Michael Lees
- Valeria V. Krzhizhanovskaya
- Jack Dongarra
- Peter M.A. Sloot
Local Organizing Committee in Zürich, Switzerland

Organizing Committee Chairs
Petros Koumoutsakos, Eleni Chatzi
Organizing Committee Members
Susanne Lewis, Maria Gião

Workshops and Organizers

Advances in High-Performance Computational Earth Sciences: Applications and Frameworks
Kengo Nakajima, Xing Cai

Agent-based Simulations, Adaptive Algorithms and Solvers
Maciej Paszynski, Robert Schaefer, Victor Calo, David Pardo

Applications of Matrix Computational Methods in the Analysis of “Modern Data”
Kourosh Modarresi

Architecture, Languages, Compilation and Hardware Support for Emerging Manycore Systems
Stéphane Louise, Loïc Cudennec, Jeronimo Castrillón, Vanía Marangozova-Martin, Martha Johanna Sepulveda Flores

Biomedical and Bioinformatics Challenges for Computer Science
Mario Cannataro, Giuseppe Agapito, Mauro Castelli, Riccardo Dondi, Italo Zoppis

Bridging the HPC Talent Gap with Computational Science Research Methods
Nia Alexandrov, Vassil Alexandrov

Computational Chemistry and Its Applications
Ponnadurai Ramasami

Computational Finance and Business Intelligence
Yong Shi, Shouyang Wang, Yingjie Tian

Computational Optimization, Modelling and Simulation
Xin-She Yang, Slawomir Koziel, Leifur Leifsson

Data-Driven Computational Sciences
Craig Douglas, Abani Patra, Ana Cortés, Robert Lodder

Environmental Computing Applications – State of the Art
Matti Heikkurinen, Dieter Kranzlmüller, Eric Yen

Large Scale Computational Physics
Elise de Doncker, Fukuko Yuasa, Tadashi Ishikawa

Mathematical Methods and Algorithms for Extreme Scale
Vassil Alexandrov, Jack Dongarra
Multiscale Modelling and Simulation
Derek Groen, Valeria Krzhizhanovskaya, Bosak Bartosz, Alfons Hoekstra, Petros Koumoutsakos

Simulations of Flow and Transport: Modeling, Algorithms and Computation
Shuyu Sun, Jianguo Liu

Solving Problems with Uncertainties
Vassil Alexandrov

Teaching Computational Science
Angela B. Shiflet, Alfredo Tirado-Ramos

Tools for Program Development and Analysis in Computational Science
Andreas Knüpfer, Arndt Bode, Karl Fürlinger, Dieter Krzanilmüller, Jens Volkert, Roland Wismüller

Urgent Computing
Alexander Boukhanovsky, Marian Bubak

Reviewers

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