The Art of Computational Science, Bridging Gaps – Forming Alloys.

Preface for ICCS 2017

Petros Koumoutsakos¹, Eleni Chatzi¹, Valeria V. Krzhizhanovskaya²,³, Michael Lees², Jack Dongarra⁴, Peter M.A. Sloot²,³,⁵

¹ETH Zürich, Switzerland
²University of Amsterdam, The Netherlands
³ITMO University, Russia
⁴University of Tennessee, USA
⁵Nanyang Technological University Singapore

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.

© 2017 The Authors. Published by Elsevier B.V.
Peer-review under responsibility of the scientific committee of the International Conference on Computational Science
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 Castrillon, Vania 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 Kranzlmüller, Jens Volkert, Roland Wismüller

Urgent Computing
Alexander Boukhanovsky, Marian Bubak

Reviewers

- David Abramson
- Giuseppe Agapito
- Ram Akella
- Elisabete Alberdi
- Marco Aldinucci
- Nia Alexandrov
- Vassil Alexandrov
- H. Ali
- Gabrielle Allen
- Ilkay Altintas
- Stanislaw Ambroszkiewicz
- Anand Amrit
- Michael Antolovich
- Joseph Antony
- Hideo Aochi
- Hamid Arabnia
- Tomasz Arodz
- Tomas Artes
- Ebrahim Bagheri
- Bartosz Balis
- Krzysztof Banas
- Bosak Bartosz
- Daniel Becker
- Jörn Behrens
- Adrian Bekasiewicz
- Gebrail Bekdas
- Adam Belloum
- Stefano Beretta
- Daniel Berrar
- John Betts
- Sanjukta Bhowmick
- Anna Bilyatdinova
- Guillaume Blin
- Alex Bokov
- Tore Brinek
- Marian Bubak
- Kris Bubendorfer
- Marcin Budka
- Jérémy Buisson
- Aleksander Byrski
- Xing Cai
- Mario Cannataro
- Junwei Cao
- Mauro Castelli
- Jeronimo Castrillon
- David Cavander
- Eduardo Cesar
- Imen Chakroun
- Eleni Chatzi
- Huangxin Chen
- Mingyang Chen
- Siew Ann Cheong
- Hongmei Chi
- Davide Chicco
- S.F. Chien
- Svetlana Chuprina
- Adriano Cortes
- Ana Cortes
- Enrique Costa-Montenegro
- Camille Coti
- Carlos Cotta
- Hélène Coullon
- Attila Csikasz-Nagy
- Loïc Cudennec
- Javier Cuenca
- Yifeng Cui
- Pawel Czarnul
- Lisandro Dalcin
- Bhaskar Dasgupta
- Susumu Date
- Raymon de Callafon
- Elise de Doncker
- Kees de Graaf
- Quanling Deng
- Xiaolong Deng
Nilanjan Dey
Louis Dijkstra
Minh Dinh
Grzegorz Dobrowolski
Riccardo Dondi
Ruggero Donida Labati
Craig C. Douglas
Rafal Drezewski
Jian Du
Xiaosong Du
Vitor Duarte
Witold Dzwinek
Nahid Emad
Christian Engelmann
Javier Espinosa
C. Filelis-Papadopoulos
Iztok Fister
Tony Ford
Geoffrey C. Fox
Muftah Fraier
Anton Frank
Karl Frinkle
Karl Fuerlinger
Wlodzimierz Funika
Takashi Furumura
Robin Gandhi
Luis Garcia-Castillo
Frédéric Gava
Zong-Woo Geem
Nils Gentschen Felde
Alexandros Gerbessiotis
Domingo Gimenez
Frank Giraldo
Christophe Giraud-Carrier
Bruno Gonçalves
Ivo Gonçalves
Yuriy Gorbachev
Pawel Gorecki
Christopher Gottbrath
George Gravvanis
Clemens Greiek
Derek Groen
Lutz Gross
Kun Guo
Piotr Gurgul
Pietro Hiram Guzzi
Diana Gähringer
Mohamed Hamada
Jeff Hammond
Dongxu Han
Mattie Heikkuinen
Alexander Heinecke
Ladislav Hluchy
Bogumiła Hnatkowska
Alfons Hoekstra
Paul Hofmann
Robert Hsu
Sascha Hunold
Tadashi Ishikawa
A. Itkin
Hideya Iwasaki
Takeshi Iwashita
Heike Jagode
Momin Jamil
Vytautas Jancauskas
Jiří Jaroš
Chao Jin
Hai Jin
David Johnson
Anshul Joshi
Xuchan Ju
Hartmut Kaiser
Ananth Kalyanaraman
George Kamps
B.D. Kandhai
Aneta Karavanova
Sven Karol
Takahiro Katagiri
Wayne Kelly
Jeremy Kepner
D. Khazanchi
Andreas Knuepfer
Waldemar Koczkodaj
Ivan Kondov
Vladimir Korkhov
Ilias Kotsireas
Jisheng Kou
Sergey Kovalchuk
Slawomir Koziel
Dieter Kranzlmüller
Valeria Krzhizhanovskaya
Jitendra Kumar
Massimo La Rosa
Anna-Lena Lamprecht
Rubin Landau
Holly Lanham
Vianney Lapotre
Jysoo Lee
Michael Lees
Leifur Leifsson
Roy Liettieri
Andrew Lewis
Jingfa Li
Hong Liu
James Liu
Marcelo Lobosco
Robert Lodder
Wen Long
Stephane Louise
Frederic Loulergue
Paul Lu
Scott MacLachlan
Akash Maharaj
Maciej Malawski
Vania Marangozova-Martín
Tomas Margalef
Tiziana Margaria
Svetozar Margenov
Osni Marques
Michael Mascagni
Marco Mattavelli
Emil Matus
Pawel Matuszyk
Valerie Maxville
Rahul Mazumder
Wagner Meira Jr.
Roderick Melnik
Ivan Merelli
John Michopoulos
Ju Ming
Kourosh Modarresi
Lampros Mountrakis
Ignacio Muga
Hiromichi Nagao
Kengo Nakajima
Philippe Navaux
Hoang Nguyen
Mai Nguyen
Sinan Melih Nigdeli
Lingfeng Niu
James Okeefe
Kenji Ono
J.P. Papa
Marcin Paprzycki
David Pardo
R.S. Parpinelli
Anna Paszynska
Maciej Paszynski
Abani Patra
Andreas Pester