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 Marangozoa-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


Gebrail Bekdas  Adam Belloum  Stefano Beretta  Daniel Berrar  John Betts  Sanjukta Bhowmick  Anna Bilyatdinova  Guillaume Blin  Alex Bokov  Tore Brinck  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 Cotillon  Attila Csikasz-Nagy  Loïc Cudennec  Javier Cuenca  Yifeng Cui  Pawel Czarnul  Lisandro Dalcin  Bhaskar Dasgupta  Susumu Date

Nilanjan Dey  Matti Heikkurinen  Roy Lettieri
Louis Dijkstra  Alexander Heinecke  Andrew Lewis
Minh Dinh  Ladislav Hluchy  Jingfa Li
Grzegorz Dobrowolski  Bogumila Hnatkowska  Hong Liu
Riccardo Dondi  Alfons Hoekstra  James Liu
Ruggiero Donida Labati  Paul Hofmann  Marcelo Lobosco
Craig C. Douglas  Robert Hsu  Robert Lodder
Rafal Drezewski  Sascha Hunold  Wen Long
Jian Du  Tadashi Ishikawa  Stephane Louise
Xiaosong Du  A. Itkin  Frederic Loulergue
Vitor Duarte  Hideya Iwasaki  Paul Lu
Witold Dzwinel  Takeshi Iwashita  Scott MacLachlan
Nahid Emad  Heike Jagode  Akash Maharaj
Christian Engelmann  Momin Jamil  Maciej Malawski
Javier Espinosa  Vytautas Jancauskas  Vania Marangozo-Martin
C. Filelis-Papadopoulos  Jiří Jaroš  Tomas Margalef
Iztok Fister  Chao Jin  Tiziana Margaria
Tony Ford  Hai Jin  Osni Marques
Geoffrey C. Fox  David Johnson  Michael Mascagni
Mustaf Fraiher  Anshul Joshi  Marco Mattavelli
Anton Frank  Xuchan Ju  Emil Matus
Karl Frinkle  Hartmut Kaiser  Pawel Matuszyk
Karl Fuerlinger  Ananth Kalyanaraman  Valerie Maxville
Wlodzimierz Funika  George Kampis  Rahul Mazumder
Takashi Furumura  B.D. Kandhai  Wagner Meira Jr.
Robin Gandhi  Aneta KARAivanova  Roderick Melnik
Luis Garcia-Castillo  Sven Karol  Ivan Merelli
Frédéric Gava  Takahiro Katagiri  John Michopoulos
Zong-Woo Geem  Wayne Kelly  Ju Ming
Nils Gentschen Felde  Jeremy Kepner  Kourosh Modarresi
Alexandros Gerbessiotis  D. Khazanchi  Lampros Mountrakis
Domingo Gimenez  Andreas Knuepper  Ignacio Muga
Frank Giraldo  Waldemar Koczokodaj  Hiromichi Nagao
Christophe Giraud-Carrier  Ivan Kondov  Kengo Nakajima
Bruno Gonçalves  Vladimir Korkhov  Philippe Navaux
Ivo Gonçalves  Ilias Kotsireas  Hoang Nguyen
Yuriy Gorbachev  Jisheng Kou  Mai Nguyen
Pawel Gorecki  Sergey Kovalchuk  Sinan Melih Nigdeli
Christopher Gottbrath  Slawomir Koziel  Lingfeng Niu
George Gravvanis  Dieter Kranzmueller  James Okeefe
Clemens GreleK  Valeria Krzhizhanovskaya  Kenji Ono
Derek Groen  Jitendra Kumar  J.P. Papa
Lutz Gross  Massimo La Rosa  Marcin Paprzycki
Kun Guo  Anna-Lena Lamprecht  David Pardo
Piotr Gurgul  Rubin Landau  R.S. Parpinelli
Pietro Hiram Guzzi  Holly Lanham  Anna Paszynska
Diana Goehringer  Vianney Lapotre  Maciej Paszynski
Mohamed Hamada  Jysoo Lee  Abani Patra
Jeff Hammond  Michael Lees  Andreas Pester
Dongxu Han  Leifur Leifsson 
<table>
<thead>
<tr>
<th>Dana Petcu</th>
<th>Bertil Schmidt</th>
<th>Pierangelo Veltri</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eric Petit</td>
<td>Alexander Schug</td>
<td>Raja Velu</td>
</tr>
<tr>
<td>Serge Petiton</td>
<td>Martin Schulz</td>
<td>Antonio M. Vidal</td>
</tr>
<tr>
<td>Daniela Piccioni</td>
<td>Martha J. Sepulveda Flores</td>
<td>David Walker</td>
</tr>
<tr>
<td>Tomasz Piontek</td>
<td>Omri Shemesh</td>
<td>Bo Wang</td>
</tr>
<tr>
<td>Erwan Piriou</td>
<td>Sameer Shende</td>
<td>Jianwu Wang</td>
</tr>
<tr>
<td>Yuri Pirola</td>
<td>Yong Shi</td>
<td>Liqiang Wang</td>
</tr>
<tr>
<td>Antoniu Pop</td>
<td>Angela Shiflet</td>
<td>Peng Wang</td>
</tr>
<tr>
<td>Marco Previtali</td>
<td>Takashi Shimokawabe</td>
<td>Shouyang Wang</td>
</tr>
<tr>
<td>Ela Pustulka-Hunt</td>
<td>Robert Sinkovits</td>
<td>Yi Wang</td>
</tr>
<tr>
<td>Vladimir Puzyrev</td>
<td>Renata Slota</td>
<td>Gregory Watson</td>
</tr>
<tr>
<td>Alexander Pyayt</td>
<td>Sucha Smanchat</td>
<td>Josef Weidendorfer</td>
</tr>
<tr>
<td>Zhiquan Qi</td>
<td>Maciej Smolka</td>
<td>Josef Weinhub</td>
</tr>
<tr>
<td>Rick Quax</td>
<td>Bartłomiej Sniezynski</td>
<td>Jens Weismüller</td>
</tr>
<tr>
<td>Waldemar Rachowicz</td>
<td>Steve Stevenson</td>
<td>Bill Williams</td>
</tr>
<tr>
<td>Ponnadurai Ramasami</td>
<td>Achim Streit</td>
<td>Roland Wismüller</td>
</tr>
<tr>
<td>Raul Ramirez</td>
<td>Barbara Strug</td>
<td>Jia Wu</td>
</tr>
<tr>
<td>Vishwas Rao</td>
<td>Bongwon Suh</td>
<td>Huilin Xing</td>
</tr>
<tr>
<td>Lukasz Rauch</td>
<td>Hailong Sun</td>
<td>Chao-Tung Yang</td>
</tr>
<tr>
<td>Alistair Rendell</td>
<td>Shuyu Sun</td>
<td>Xin-She Yang</td>
</tr>
<tr>
<td>Alistair Reveill</td>
<td>James Suter</td>
<td>Eric Yen</td>
</tr>
<tr>
<td>Jason Riedy</td>
<td>Martin Swain</td>
<td>Xiaodan Yu</td>
</tr>
<tr>
<td>Sophie Robert</td>
<td>Ryszard Tadeusiewicz</td>
<td>Hongyuan Yuan</td>
</tr>
<tr>
<td>Yves Robert</td>
<td>Daisuke Takahashi</td>
<td>Fukuko Yuasa</td>
</tr>
<tr>
<td>Daniel Rodriguez</td>
<td>Osamu Tatebe</td>
<td>Qi Zeng</td>
</tr>
<tr>
<td>Albert Romkes</td>
<td>Andrei Tchernykh</td>
<td>H. Zhang</td>
</tr>
<tr>
<td>Debraj Roy</td>
<td>Cedric Tedeschi</td>
<td>Qin Zhang</td>
</tr>
<tr>
<td>Justin Ruths</td>
<td>Tamás Terlaky</td>
<td>Yao Zhang</td>
</tr>
<tr>
<td>Katarzyna Rycerz</td>
<td>Yonatan A. Tesfahunegn</td>
<td>Hua Zhong</td>
</tr>
<tr>
<td>Ali Sadollah</td>
<td>Andrew Thelen</td>
<td>Jinghui Zhong</td>
</tr>
<tr>
<td>Fahad Saeed</td>
<td>Yingjie Tian</td>
<td>Xiaofei Zhou</td>
</tr>
<tr>
<td>Alberto Sanchez</td>
<td>T.O. Ting</td>
<td>Sotirios Ziavras</td>
</tr>
<tr>
<td>Hitoshi Sato</td>
<td>Alfredo Tirado-Ramos</td>
<td>Andrea Zonca</td>
</tr>
<tr>
<td>Robert Schaefer</td>
<td>Paolo Trunfio</td>
<td>Italo Zoppis</td>
</tr>
<tr>
<td>Olaf Schenk</td>
<td>Pavel Tvrdik</td>
<td>Grażyna Ślusarczyk</td>
</tr>
<tr>
<td>Ulf D. Schiller</td>
<td>Bora Ucar</td>
<td></td>
</tr>
</tbody>
</table>