The Art of Computational Science, Bridging Gaps - Forming Alloys
Preface for ICCS 2017
Koumoutsakos, P.; Chatzi, E.; Krzhizhanovskaya, V.V.; Lees, M.; Dongarra, J.; Sloot, Peter M.A.
DOI
10.1016/j.procs.2017.05.281
Publication date
2017
Document Version
Final published version
Published in
Procedia Computer Science
License
CC BY-NC-ND
Link to publication

Citation for published version (APA):
https://doi.org/10.1016/j.procs.2017.05.281

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: https://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.

UvA-DARE is a service provided by the library of the University of Amsterdam (https://dare.uva.nl)
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

<table>
<thead>
<tr>
<th>Name</th>
<th>Name</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>David Abramson</td>
<td>Gebrail Bekdas</td>
<td>Mingyang Chen</td>
</tr>
<tr>
<td>Giuseppe Agapito</td>
<td>Adam Belloum</td>
<td>Siew Ann Cheong</td>
</tr>
<tr>
<td>Ram Akella</td>
<td>Stefano Beretta</td>
<td>Hongmei Chi</td>
</tr>
<tr>
<td>Elisabete Alberdi</td>
<td>Daniel Berrar</td>
<td>Davide Chicco</td>
</tr>
<tr>
<td>Marco Aldinucci</td>
<td>John Betts</td>
<td>S.F. Chien</td>
</tr>
<tr>
<td>Nia Alexandrov</td>
<td>Sanjukta Bhowmick</td>
<td>Svetlana Chuprina</td>
</tr>
<tr>
<td>Vassil Alexandrov</td>
<td>Anna Bilyatdinova</td>
<td>Adriano Cortes</td>
</tr>
<tr>
<td>H. Ali</td>
<td>Guillaume Blin</td>
<td>Ana Cortes</td>
</tr>
<tr>
<td>Gabrielle Allen</td>
<td>Alex Bokov</td>
<td>Enrique Costa-Montenegro</td>
</tr>
<tr>
<td>Ilkay Altintas</td>
<td>Tore Brinck</td>
<td>Camille Coti</td>
</tr>
<tr>
<td>Stanislaw Ambroszkiewicz</td>
<td>Marian Bubak</td>
<td>Carlos Cotta</td>
</tr>
<tr>
<td>Anand Amrit</td>
<td>Kris Bubendorfer</td>
<td>Hélène Cotillon</td>
</tr>
<tr>
<td>Michael Antolovich</td>
<td>Marcin Budka</td>
<td>Attila Csikasz-Nagy</td>
</tr>
<tr>
<td>Joseph Antony</td>
<td>Jérémy Buisson</td>
<td>Loïc Cudennec</td>
</tr>
<tr>
<td>Hideo Aochi</td>
<td>Aleksander Byrski</td>
<td>Javier Cuenca</td>
</tr>
<tr>
<td>Hamid Arabnia</td>
<td>Xing Cai</td>
<td>Yifeng Cui</td>
</tr>
<tr>
<td>Tomasz Arodz</td>
<td>Mario Cannataro</td>
<td>Pawel Czarnul</td>
</tr>
<tr>
<td>Tomas Artes</td>
<td>Junwei Cao</td>
<td>Lisandro Dalcin</td>
</tr>
<tr>
<td>Ebrahim Bagheri</td>
<td>Mauro Castelli</td>
<td>Bhaskar Dasgupta</td>
</tr>
<tr>
<td>Bartosz Balis</td>
<td>Jeronimo Castrillon</td>
<td>Susumu Date</td>
</tr>
<tr>
<td>Krzysztof Banas</td>
<td>David Cavander</td>
<td>Raymond de Callafon</td>
</tr>
<tr>
<td>Bosak Bartosz</td>
<td>Eduardo Cesar</td>
<td>Elise de Doncker</td>
</tr>
<tr>
<td>Daniel Becker</td>
<td>Imen Chakroun</td>
<td>Kees de Graaf</td>
</tr>
<tr>
<td>Jörn Behrens</td>
<td>Eleni Chatzi</td>
<td>Quanling Deng</td>
</tr>
<tr>
<td>Adrian Bekasiewicz</td>
<td>Huangxin Chen</td>
<td>Xiaolong Deng</td>
</tr>
</tbody>
</table>
Nilanjan Dey
Louis Dijkstra
Minh Dinh
Grzegorz Dobrowolski
Riccardo Dondi
Ruggiero Donida Labati
Craig C. Douglas
Rafal Drezewski
Jian Du
Xiaosong Du
Vitor Duarte
Witold Dzwiel
Nahid Emad
Christian Engelmann
Javier Espinosa
C. Filelis-Papadopoulos
Iztok Fister
Tony Ford
Geoffrey C. Fox
Muftah Fraiber
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 Grelek
Derek Groen
Lutz Gross
Kun Guo
Piotr Gurgul
Pietro Hiram Guzzi
Diana Göhringer
Mohamed Hamada
Jeff Hammond
Dongxu Han
Matt Heikkurinen
Alexander Heinecke
Ladislav Hluchy
Bogumila Hnatkowska
Alfons Hoekstra
Paul Hofmann
Robert Hsu
Sascha Hunold
Tadashi Ishikawa
A. Itkin
Hideya Iwasaki
Takeshi Iwashita
Heike Jagode
Momin Jamil
Vytautas Jancauskas
Jiří Jaros
Chao Jin
Hai Jin
David Johnson
Anshul Joshi
Xuchan Ju
Hartmut Kaiser
Ananth Kalyanaraman
George Kampis
B.D. Kandhai
Aneta Karaivanova
Sven Karol
Takahiro Katagiri
Wayne Kelly
Jeremy Kepner
D. Khazanchi
Andreas Knueper
Waldemar Koczkodaj
Ivan Kondov
Vladimir Korkhov
IIias 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 Lettieri
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-Martin
Tomas Margalef
Tiziana Margaria
Svetozar Marginov
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
Dana Petcu
Eric Petit
Serge Petiton
Daniela Piccioni
Tomasz Piontek
Erwan Piriou
Yuri Pirola
Antoniou Pop
Marco Previtali
Ela Pustulka-Hunt
Vladimir Puzyrev
Alexander Pyayt
Zhiquan Qi
Rick Quax
Waldemar Rachowicz
Ponnadurai Ramasami
Raul Ramirez
Vishwas Rao
Lukasz Rauch
Alistair Rendell
Alistair Revell
Jason Riedy
Sophie Robert
Yves Robert
Daniel Rodriguez
Albert Romkes
Debraj Roy
Justin Ruths
Katarzyna Rycerz
Ali Sadollah
Fahad Saeed
Alberto Sanchez
Hitoshi Sato
Robert Schaefer
Olaf Schenk
Ulf D. Schiller
Bertil Schmidt
Alexander Schug
Martin Schulz
Martha J. Sepulveda Flores
Omri Shemes
Sameer Shende
Yong Shi
Angela Shiflet
Takashi Shimokawabe
Robert Sinkovits
Renata Slota
Sucha Smanchat
Maciej Smolka
Bartłomiej Snieczynski
Steve Stevenson
Achim Streit
Barbara Strug
Bongwon Suh
Haibin Sun
Shuyu Sun
James Suter
Martin Swain
Ryszard Tadeusiewicz
Daisuke Takahashi
Osamu Tatebe
Andrei Tchernykh
Cedric Tedeschi
Tamás Terlaky
Yonatan A. Tesfahunegn
Andrew Thelen
Yingjie Tian
T.O. Ting
Alfredo Tirado-Ramos
Paolo Trunfio
Pavel Tvrdik
Bora Ucar
Pierangelo Veltri
Raja Velu
Antonio M. Vidal
David Walker
Bo Wang
Jianwu Wang
Liqiang Wang
Peng Wang
Shouyang Wang
Yi Wang
Gregory Watson
Josef Weidendorfer
Josef Weinhub
Jens Weismüller
Bill Williams
Roland Wismüller
Jia Wu
Huilin Xing
Chao-Tung Yang
Xin-She Yang
Eric Yen
Xiaodan Yu
Hongyuan Yuan
Fukuko Yuasa
Qi Zeng
H. Zhang
Qin Zhang
Yao Zhang
Hua Zhong
Jinghui Zhong
Xiaofei Zhou
Sotirios Ziavras
Andrea Zonca
Italo Zoppis
Grażyna Ślusarczyk