



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

Petros Koumoutsakos¹, Eleni Chatzi¹, Valeria V. Krzhizhanovskaya^{2,3},
Michael Lees², Jack Dongarra⁴, Peter M.A. Sloot^{2,3,5}

¹*ETH Zürich, Switzerland*

²*University of Amsterdam, The Netherlands*

³*ITMO University, Russia*

⁴*University of Tennessee, USA*

⁵*Nanyang 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 *Intelligibilis* 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
Organizing Committee Members

Petros Koumoutsakos, Eleni Chatzi
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 Furlinger, Dieter Kranzlmüller, Jens Volkert, Roland Wismüller

Urgent Computing

Alexander Boukhanovsky, Marian Bubak

Reviewers

David Abramson	Gebrail Bekdas	Mingyang Chen
Giuseppe Agapito	Adam Belloum	Siew Ann Cheong
Ram Akella	Stefano Beretta	Hongmei Chi
Elisabete Alberdi	Daniel Berrar	Davide Chicco
Marco Aldinucci	John Betts	S.F. Chien
Nia Alexandrov	Sanjukta Bhowmick	Svetlana Chuprina
Vassil Alexandrov	Anna Bilyatdinova	Adriano Cortes
H. Ali	Guillaume Blin	Ana Cortes
Gabrielle Allen	Alex Bokov	Enrique Costa-Montenegro
Ilkay Altintas	Tore Brinck	Camille Coti
Stanislaw Ambroszkiewicz	Marian Bubak	Carlos Cotta
Anand Amrit	Kris Bubendorfer	Hélène Coullon
Michael Antolovich	Marcin Budka	Attila Csikasz-Nagy
Joseph Antony	Jérémy Buisson	Loïc Cudennec
Hideo Aochi	Aleksander Byrski	Javier Cuenca
Hamid Arabnia	Xing Cai	Yifeng Cui
Tomasz Arodz	Mario Cannataro	Pawel Czarnul
Tomas Artes	Junwei Cao	Lisandro Dalcin
Ebrahim Bagheri	Mauro Castelli	Bhaskar Dasgupta
Bartosz Balis	Jeronimo Castrillon	Susumu Date
Krzysztof Banas	David Cavander	Raymond de Callafon
Bosak Bartosz	Eduardo Cesar	Elise de Doncker
Daniel Becker	Imen Chakroun	Kees de Graaf
Jörn Behrens	Eleni Chatzi	Quanling Deng
Adrian Bekasiewicz	Huangxin Chen	Xiaolong Deng

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
Ruggero 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
Christatian Engelmann	Momin Jamil	Maciej Malawski
Javier Espinosa	Vytautas Jancauskas	Vania Marangozova-Martin
C. Filelis-Papadopoulos	Jiří Jaroš	Tomas Margalef
Iztok Fister	Chao Jin	Tiziana Margaria
Tony Ford	Hai Jin	Svetozar Margenov
Geoffrey C. Fox	David Johnson	Osni Marques
Muftah Fraifer	Anshul Joshi	Michael Mascagni
Anton Frank	Xuchan Ju	Marco Mattavelli
Karl Frinkle	Hartmut Kaiser	Emil Matus
Karl Fuerlinger	Ananth Kalyanaraman	Pawel Matuszyk
Wlodzimierz Funika	George Kampis	Valerie Maxville
Takashi Furumura	B.D. Kandhai	Rahul Mazumder
Robin Gandhi	Aneta Karaivanova	Wagner Meira Jr.
Luis Garcia-Castillo	Sven Karol	Roderick Melnik
Frédéric Gava	Takahiro Katagiri	Ivan Merelli
Zong-Woo Geem	Wayne Kelly	John Michopoulos
Nils Gentschen Felde	Jeremy Kepner	Ju Ming
Alexandros Gerbessiotis	D. Khazanchi	Kourosh Modarresi
Domingo Gimenez	Andreas Kneuper	Lampros Mountrakis
Frank Giraldo	Waldemar Koczkodaj	Ignacio Muga
Christophe Giraud-Carrier	Ivan Kondov	Hiromichi Nagao
Bruno Gonçalves	Vladimir Korkhov	Kengo Nakajima
Ivo Gonçalves	Ilias Kotsireas	Philippe Navaux
Yuriy Gorbachev	Jisheng Kou	Hoang Nguyen
Pawel Gorecki	Sergey Kovalchuk	Mai Nguyen
Christopher Gottbrath	Slawomir Koziel	Sinan Melih Nigdeli
George Gravvanis	Dieter Kranzlmüller	Lingfeng Niu
Clemens Grelck	Valeria Krzhizhanovskaya	James Okeeffe
Derek Groen	Jitendra Kumar	Kenji Ono
Lutz Gross	Massimo La Rosa	J.P. Papa
Kun Guo	Anna-Lena Lamprecht	Marcin Paprzycki
Piotr Gurgul	Rubin Landau	David Pardo
Pietro Hiram Guzzi	Holly Lanham	R.S. Parpinelli
Diana Göhringer	Vianney Lapotre	Anna Paszynska
Mohamed Hamada	Jysoo Lee	Maciej Paszynski
Jeff Hammond	Michael Lees	Abani Patra
Dongxu Han	Leifur Leifsson	Andreas Pester

Dana Petcu	Bertil Schmidt	Pierangelo Veltri
Eric Petit	Alexander Schug	Raja Velu
Serge Petiton	Martin Schulz	Antonio M. Vidal
Daniela Piccioni	Martha J. Sepulveda Flores	David Walker
Tomasz Piontek	Omri Shemesh	Bo Wang
Erwan Piriou	Sameer Shende	Jianwu Wang
Yuri Pirola	Yong Shi	Liqiang Wang
Antoni Pop	Angela Shiflet	Peng Wang
Marco Previtali	Takashi Shimokawabe	Shouyang Wang
Ela Pustulka-Hunt	Robert Sinkovits	Yi Wang
Vladimir Puzyrev	Renata Slota	Gregory Watson
Alexander Pyayt	Sucha Smachat	Josef Weidendorfer
Zhiquan Qi	Maciej Smółka	Josef Weinbub
Rick Quax	Bartłomiej Sniezynski	Jens Weismüller
Waldemar Rachowicz	Steve Stevenson	Bill Williams
Ponnadurai Ramasami	Achim Streit	Roland Wismüller
Raul Ramirez	Barbara Strug	Jia Wu
Vishwas Rao	Bongwon Suh	Huilin Xing
Lukasz Rauch	Hailong Sun	Chao-Tung Yang
Alistair Rendell	Shuyu Sun	Xin-She Yang
Alistair Revell	James Suter	Eric Yen
Jason Riedy	Martin Swain	Xiaodan Yu
Sophie Robert	Ryszard Tadeusiewicz	Hongyuan Yuan
Yves Robert	Daisuke Takahashi	Fukuko Yuasa
Daniel Rodriguez	Osamu Tatebe	Qi Zeng
Albert Romkes	Andrei Tchernykh	H. Zhang
Debraj Roy	Cedric Tedeschi	Qin Zhang
Justin Ruths	Tamás Terlaky	Yao Zhang
Katarzyna Rycerz	Yonatan A. Tesfahunegn	Hua Zhong
Ali Sadollah	Andrew Thelen	Jinghui Zhong
Fahad Saeed	Yingjie Tian	Xiaofei Zhou
Alberto Sanchez	T.O. Ting	Sotirios Ziafras
Hitoshi Sato	Alfredo Tirado-Ramos	Andrea Zonca
Robert Schaefer	Paolo Trunfio	Italo Zoppis
Olaf Schenk	Pavel Tvrdik	Grażyna Ślusarczyk
Ulf D. Schiller	Bora Ucar	