

Computational Science for a Better Future.

Preface to ICCS 2021

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1. Introduction

Welcome to the 21st annual International Conference on Computational Science (ICCS - <https://www.iccs-meeting.org/iccs2021/>).

In preparing this edition, we had high hopes that the ongoing pandemic would fade away and allow us to meet this June in the beautiful city of Kraków. Unfortunately, such is not yet the case, as the world struggles to adapt to the many profound changes brought about by this crisis. ICCS 2021 has had to adapt too and is thus being held entirely online, for the first time in its history.

These challenges notwithstanding, we have tried our best to keep the ICCS community as dynamic and productive as always. We are proud to present the proceedings you are reading as a result of that.

ICCS 2021 is jointly organized by the AGH University of Science and Technology, the 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, as well as researchers from various application areas who are pioneering computational methods in sciences such as physics, chemistry, life sciences, engineering, arts, and humanitarian fields, to discuss problems and solutions in the area, identify new issues, and 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 350 expected participants. The proceedings series have become a primary intellectual resource for computational science researchers, defining and advancing the state-of-the-art in this field.

The theme for 2021, "**Computational Science for a Better Future**," highlights the role of Computational Science in tackling the current challenges of our fast-changing world. 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 physical systems, computational and systems biology, environmental systems, finance, and others.

ICCS is well known for its excellent lineup of keynote speakers. The keynotes for 2021 are:

- **Maciej Besta**, ETH Zürich, Switzerland
- **Marian Bubak**, AGH University of Science and Technology, Poland | Sano Centre for Computational Medicine, Poland
- **Anne Gelb**, Dartmouth College, USA
- **Georgiy Stenchikov**, King Abdullah University of Science and Technology, Saudi Arabia
- **Marco Viceconti**, University of Bologna, Italy
- **Krzysztof Walczak**, Poznan University of Economics and Business, Poland
- **Jessica Zhang**, Carnegie Mellon University, USA

This year we had 635 submissions (156 submissions to the main track and 479 to the thematic tracks). In the main track, 48 full papers were accepted (31%); in the thematic tracks, 212 full papers (44%). A high acceptance rate in the thematic tracks is explained by the nature of these, where track organisers personally invite many experts in a particular field to participate in their sessions.

ICCS relies strongly on our thematic track organizers' vital contributions to attract high-quality papers in many subject areas. We would like to thank all committee members from the main and thematic tracks for their contribution to ensure a high standard for the accepted papers. We would also like to thank *Springer*, *Elsevier*, and *Intelligibilis* for their support. Finally, we appreciate all the local organizing committee members for their hard work to prepare for this conference.

We are proud to note that ICCS is an A-rank conference in the CORE classification.

We wish you good health in these troubled times and look forward to meeting you at the conference.

June 2021

The ICCS 2021 Organizers:

Maciej Paszynski
Dieter Kranzlmüller
Valeria V. Krzhizhanovskaya
Jack J. Dongarra
Peter M.A. Sloot

2. Local Organizing Committee at AGH University of Science and Technology

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3. Thematic Tracks and Organizers

Advances in High-Performance Computational Earth Sciences: Applications and Frameworks – IHPCES

Takashi Shimokawabe, Kohei Fujita, Dominik Bartuschat

Applications of Computational Methods in Artificial Intelligence and Machine Learning – ACMAIML

Kourosh Modarresi, Paul Hofmann, Raja Velu, Peter Woehrmann

Artificial Intelligence and High-Performance Computing for Advanced Simulations – AIHPC4AS

Maciej Paszynski, Robert Schaefer, David Pardo, Victor Calo

Biomedical and Bioinformatics Challenges for Computer Science – BBC

Mario Cannataro, Giuseppe Agapito, Mauro Castelli, Riccardo Dondi, Italo Zoppis

Classifier Learning from Difficult Data – CLD²

Michał Woźniak, Bartosz Krawczyk

Computational Analysis of Complex Social Systems – CSOC

Debraj Roy

Computational Collective Intelligence – CCI

Marcin Maleszka, Ngoc Thanh Nguyen, Marcin Hernes, Sinh Van Nguyen

Computational Health – CompHealth

Sergey Kovalchuk, Georgiy Bobashev, Stefan Thurner

Computational Methods for Emerging Problems in (dis-)Information Analysis – DisA

Michał Choras, Robert Burduk, Konstantinos Demestichas

Computational Methods in Smart Agriculture – CMSA

Andrew Lewis

Computational Optimization, Modelling, and Simulation – COMS

Xin-She Yang, Leifur Leifsson, Slawomir Koziel

Computational Science in IoT and Smart Systems – IoTSS

Vaidy Sunderam, Dariusz Mrozek

Computer Graphics, Image Processing and Artificial Intelligence – CGIPAI

Andres Iglesias, Lihua You, Alexander Malyshev, Hassan Ugail

Data-Driven Computational Sciences – DDCS

Craig Douglas

Machine Learning and Data Assimilation for Dynamical Systems – MLDADS

Rossella Arcucci

MeshFree Methods and Radial Basis Functions in Computational Sciences – MESHFREE

Vaclav Skala, Marco-Evangelos Biancolini, Samsul Ariffin Abdul Karim, Rongjiang Pan, Fernando-César Meira-Menandro

Multiscale Modelling and Simulation – MMS

Derek Groen, Diana Suleimenova, Stefano Casarin, Bartosz Bosak, Wouter Edeling

Quantum Computing Workshop – QCW

Katarzyna Rycerz, Marian Bubak

Simulations of Flow and Transport: Modeling, Algorithms and Computation – SOFTMAC

Shuyu Sun, Jingfa Li, James Liu

Smart Systems: Bringing Together Computer Vision, Sensor Networks and Machine Learning – SmartSys

Pedro Cardoso, Roberto Lam, João Rodrigues, Jânio Monteiro

Software Engineering for Computational Science – SE4Science

Jeffrey Carver, Neil Chue Hong, Anna-Lena Lamprecht

Solving Problems with Uncertainty – SPU

Vassil Alexandrov, Aneta Karaivanova

Teaching Computational Science – WTCS

Angela Shiflet, Nia Alexandrov, Alfredo Tirado-Ramos

Uncertainty Quantification for Computational Models – UNEQUIvOCAL

Wouter Edeling, Anna Nikishova

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