Preface

Welcome to the 24th International Conference on Computational Science (ICCS - https://www.iccs-meeting.org/iccs2024/), held on July 2-4, 2024 at the University of Málaga, Spain.

In keeping with the new normal of our times, ICCS featured both in-person and online sessions. Although the challenges of such a hybrid format are manifold, we have always tried our best to keep the ICCS community as dynamic, creative, and productive as possible. We are proud to present the proceedings you are reading as a result.

ICCS 2024 was jointly organized by the University of Málaga, the University of Amsterdam, and the University of Tennessee.

Facing the Mediterranean in Spain's Costa del Sol, Málaga is the country's sixth largest city, and a major hub for finance, tourism and technology in the region.

The University of Málaga (Universidad de Málaga – UMA) is a modern, public university, offering 63 degrees and 120 post-graduate degrees. Close to 40.000 students are studying at UMA, taught by 2500 teachers, distributed over 81 departments and 19 centers. The UMA has 278 research groups, which are involved in 80 national projects and 30 European and International projects. ICCS took place at the Teatinos Campus, home to the School of Computer Science and Engineering (ETSI Informática), which is a pioneer in its field and offers the widest range of IT-related subjects in the region of Andalusia.

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.

The ICCS proceedings series have become a primary intellectual resource for computational science researchers, defining and advancing the state of the art in this field.

We are proud to note that this 24th edition, with 17 tracks (16 thematic tracks and one main track) and close to 300 participants, has kept to the tradition and high standards of previous editions.

The theme for 2024, " **Computational Science: Guiding the Way Towards a Sustainable Society**", highlights the role of Computational Science in assisting multidisciplinary research on sustainable solutions. This conference was 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 2024 were:

- **David Abramson**, The University of Queensland, Australia
- **Manuel Castro Díaz**, University of Málaga, Spain
- **Jiří Mikyška**, Czech Technical University in Prague, Czechia
- **Takemasa Miyoshi**, RIKEN, Japan
- **Coral Calero Muñoz**, University of Castilla-La Mancha, Spain
- **Petra Ritter**, Berlin Institute of Health & Charité University Hospital Berlin, Germany

This year we had 406 submissions (149 to the main track and 257 to the thematic tracks). In the main track, 51 full papers were accepted (34.2 %); in the thematic tracks, 104 full papers (40.5 %). A higher acceptance rate in the thematic tracks is explained by their particular nature, whereby track organizers personally invite many experts in the field to participate. Each submission received at least 2 single-blind reviews (2.8 reviews per paper on average).

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 ensuring a high standard for the accepted papers. We would also like to thank *Springer, Elsevier,* and *Intellegibilis* for their support. Finally, we appreciate all the local organizing committee members for their hard work in preparing this conference.

We hope you enjoyed the conference, whether virtually or in person.

July 2024

1. Organization

The Conference Chairs

General Chair: Valeria Krzhizhanovskaya (University of Amsterdam, The Netherlands)

Main Track Chair: Clélia de Mulatier (University of Amsterdam, The Netherlands)

Thematic Tracks Chair: Maciej Paszynski (AGH University of Krakow, Poland)

Thematic Tracks Vice Chair: Michael Harold Lees (University of Amsterdam, The Netherlands)

Scientific Chairs:
Peter M.A. Sloot (University of Amsterdam, The Netherlands)
Jack Dongarra (University of Tennessee, USA)

Local Organizing Committee @ University of Málaga

LOC Chair: Leonardo Franco

LOC Members:
Francisco Ortega-Zamorano
Francisco J. Moreno-Barea
José L. Subirats-Contreras

2. Thematic Tracks and Organizers

Advances in High-Performance Computational Earth Sciences: Numerical Methods, Frameworks & Applications– IHPCES
> Takashi Shimokawabe (The University of Tokyo, Japan)
> Kohei Fujita (The University of Tokyo, Japan)
> Dominik Bartuschat (FAU Erlangen-Nuernberg, Germany)

Artificial Intelligence and High-Performance Computing for Advanced Simulations – AIHPC4AS
> Maciej Paszynski (AGH University of Krakow, Poland)

Biomedical and Bioinformatics Challenges for Computer Science – BBC

Mario Cannataro (University Magna Graecia of Catanzaro, Italy)
Giuseppe Agapito (University Magna Graecia of Catanzaro, Italy)
Mauro Castelli (Universidade Nova de Lisboa, Portugal)
Riccardo Dondi (University of Bergamo, Italy)
Rodrigo Weber dos Santos (Federal University of Juiz de Fora, Brazil)
Italo Zoppis (University Milano-Bicocca, Italy)

Computational Diplomacy and Policy – CoDiP

Roland Bouffanais (University of Geneva, Switzerland)
Michael Lees (University of Amsterdam, The Netherlands)
Brian Castellani (Durham University, UK)

Computational Health – CompHealth

Sergey Kovalchuk (Huawei)
Georgiy Bobashev (RTI International)
Anastasia Angelopoulou (University of Westminster, UK)
Jude Hemanth (Karunya University, India)

Computational Optimization, Modelling, and Simulation – COMS

Xin-She Yang (Middlesex University London, UK)
Slawomir Koziel (Reykjavik University, Iceland)
Leifur Leifsson (Purdue University, USA)

Generative AI and Large Language Models (LLMs) in Advancing Computational Medicine – CMGAI

Ahmed Abdeen Hamed (State University of New York at Binghamton, USA)
Qiao Jin (National Institutes of Health, USA)
Xindong Wu (Hefei University of Technology, China)
Byung Lee (University of Vermont, USA)
Zhiyong Lu (National Institutes of Health, USA)
Karin Verspoor (RMIT University, Australia)
Christopher Savoie (Zapata AI, USA)

Machine Learning and Data Assimilation for Dynamical Systems – MLDADS

Rossella Arcucci (Imperial College London, UK)
Cesar Quilodran-Casas (Imperial College London, UK)

Multiscale Modelling and Simulation – MMS

Derek Groen (Brunel University London, UK)
Diana Suleimenova (Brunel University London, UK)

Network Models and Analysis: From Foundations to Artificial Intelligence – NMAI

Marianna Milano (Università Magna Graecia Catanzaro, Italy)
Giuseppe Agapito (University Magna Graecia of Catanzaro, Italy)
Pietro Cinaglia (University Magna Graecia of Catanzaro, Italy)
Chiara Zucco (University Magna Graecia of Catanzaro, Italy)

Numerical Algorithms and Computer Arithmetic for Computational Science – NACA
Pawel Gepner (Warsaw Technical University, Poland)
Ewa Deelman (University of Southern California, Marina del Rey, USA)
Hatem Ltaief (Extreme Computing Research Center, KAUST, Saudi Arabia)

Quantum Computing – QCW
Katarzyna Rycerz (AGH University of Krakow, Poland)
Marian Bubak (Sano and AGH, Poland)

Simulations of Flow and Transport: Modeling, Algorithms, and Computation – SOFTMAC
Shuyu Sun (King Abdullah University of Science and Technology, Saudi Arabia)
Jingfa Li (Beijing Institute of Petrochemical Technology, China)
James Liu (Colorado State University, USA)

Smart Systems: Bringing Together Computer Vision, Sensor Networks and Artificial Intelligence – SmartSys
Pedro Cardoso (University of Algarve, Portugal)
João Rodrigues (University of Algarve, Portugal)
Jânio Monteiro (University of Algarve, Portugal)
Roberto Lam (University of Algarve, Portugal)

Solving Problems with Uncertainties – SPU
Vassil Alexandrov (Hartree Centre - STFC, UK)
Aneta Karaivanova (IICT-Bulgarian Academy of Science, Bulgaria)

Teaching Computational Science – WTCS
Evguenia Alexandrova (Hartree Centre - STFC, UK)
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