ICCS 2023

23rd International Conference on Computational Science

Czech Technical University in Prague

Czechia | July 3-5

CTU

CZECH TECHNICAL UNIVERSITY IN PRAGUE

http://www.iccs-meeting.org/iccs2023/
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Foreword

Welcome to the 23rd annual International Conference on Computational Science (ICCS - https://www.iccs-meeting.org/iccs2023/), held on July 3-5, 2023 at the Czech Technical University in Prague, Czechia.

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.

This Book of Abstracts lists the abstracts of all papers presented at ICCS, organized by track and then by session as per the official schedule.

ICCS 2023 was jointly organized by the Czech Technical University in Prague, the University of Amsterdam, NTU Singapore, and the University of Tennessee.

Standing on the Vltava River, Prague is central Europe's political, cultural, and economic hub.

The Czech Technical University in Prague (CTU) is one of Europe's largest and oldest technical universities and the highest-rated in the group of Czech technical universities. CTU offers 350 accredited study programs, 100 of which are taught in a foreign language. Close to 19,000 students are studying at CTU in 2022/2023. The Faculty of Nuclear Sciences and Physical Engineering (FNSPE), located along the river bank in Prague's beautiful Old Town (Staré Mesto) and host to ICCS 2023, is the only one in Czechia to offer studies in a broad range of fields related to Nuclear Physics and Engineering. The Faculty operates both fission (VR-1) and fusion (GOLEM Tokamak) reactors and hosts several cutting-edge research projects, collaborating with a number of international research centers (CERN, ITER, BNL-STAR, ELI).

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 attendees and papers, and this year is not an exception, with over 300 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 2023, "**Computation at the Cutting Edge of Science**", highlights the role of Computational Science in assisting multidisciplinary research. 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 2023 were:

Helen Brooks, United Kingdom Atomic Energy Authority (UKAEA), UK

Jack Dongarra, University of Tennessee, USA

Derek Groen, Brunel University London, UK

Anders Dam Jensen, European High Performance Computing Joint Undertaking (EuroHPC JU), Luxembourg

Jakub Šístek, Institute of Mathematics of the Czech Academy of Sciences & Czech Technical University in Prague, Czechia

This year we had 531 submissions (176 to the main track and 355 to the thematic tracks). In the main track, 54 full papers were accepted (30.7 %); in the thematic tracks, 134 full papers (37.7 %). A higher acceptance rate in the thematic tracks is explained by the nature of these, where track organizers personally invite many experts in a particular field to participate in their sessions. Each submission received at least 2 single-blind reviews (2.9 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 for this conference.

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

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

The Organizers

The Conference Chairs

General Conference 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 Science and Technology, Poland

Scientific Chairs
Peter M.A. Sloot, University of Amsterdam, The Netherlands | Complexity Institute NTU, Singapore
Jack Dongarra, University of Tennessee, USA

Local Organizing Committee @ Czech Technical University in Prague

Chair
Jiří Mikyška - LOC Chair

Members
Pavel Eichler
Radek Fučík
Jakub Klinkovský
Tomáš Oberhuber
Pavel Strachota

List of Thematic Tracks and Organizers

Advances in High-Performance Computational Earth Sciences: Applications and Frameworks – IHPCESl
Takashi Shimokawabe, Kohei Fujita, Dominik Bartuschat

Artificial Intelligence and High-Performance Computing for Advanced Simulations – AIHPC4AS
Maciej Paszynski, Robert Schaefer, Victor Calo, David Pardo, Quanling Deng

Biomedical and Bioinformatics Challenges for Computer Science – BBC
Mario Cannataro, Giuseppe Agapito, Mauro Castelli, Riccardo Dondi, Rodrigo Weber dos Santos, Italo Zoppis

Computational Collective Intelligence – CCI
Marcin Maleszka, Ngoc Thanh Nguyen

Computational Diplomacy and Policy – CoDiP
Michael Lees, Brian Castellani, Bastien Chopard

Computational Health – CompHealth
Sergey Kovalchuk, Georgiy Bobashev, Anastasia Angelopoulou, Jude Hemanth

Computational Modelling of Cellular Mechanics – CMCM
Gabor Zavodszky, Igor Pivkin

Computational Optimization, Modelling, and Simulation – COMS
Xin-She Yang, Slawomir Koziel, Leifur Leifsson

Computational Social Complexity – CSCx
Vítor V. Vasconcelos. Debraj Roy, Elisabeth Krüger, Flávio Pinheiro, Alexander J. Stewart, Victoria Garibay, Andreia Sofia Teixeira, Yan Leng, Gabor Zavodszky

Computer Graphics, Image Processing, and Artificial Intelligence – CGIPAI
Andres Iglesias, Lihua You, Akemi Galvez-Tomida

Machine Learning and Data Assimilation for Dynamical Systems – MLDADS
Rossella Arcucci, Cesar Quilodran-Casas

MeshFree Methods and Radial Basis Functions in Computational Sciences – MESHFREE
Vaclav Skala, Samsul Ariffin Abdul Karim

Multiscale Modelling and Simulation – MMS
Derek Groen, Diana Suleimenova

Outlier detection under False Omission Rate control

Jan Mielniczuk and Adam Wawrzenczyk

Abstract. We argue that in many practical situations control of False Omission Rate (FOR) or Bayesian False Omission Rate (BFOR) is of primary importance. We develop and investigate such rule in the context of outlier detection, and propose its empirical formulation for practical use. We consider several score statistics used to detect outliers and study how well the introduced method controls FOR in practice. It is shown by analysis of several datasets that FOR control in contrast to FDR control is inherently tied to performance of the score statistic employed on both inlier and outlier data sets.

Symbolic-Numeric Computation in Modeling the Dynamics of the Many-Body System TRAPPIST

Alexander Chichurin, Alexander Prokopenya, Mukhtar Minglibayev and Aiken Kosherbayeva

Abstract. Modeling the dynamics of the exoplanetary system TRAPPIST with seven bodies of variable mass moving around a central parent star along quasi-elliptic orbits is discussed. The bodies are assumed to be spherically symmetric and attract each other according to Newton's law of gravitation. In this case, the leading factor of dynamic evolution of the system is the variability of the masses of all bodies. The problem is analyzed in the framework of Hamiltonian's formalism and the differential equations of motion of the bodies are derived in terms of the osculating elements of aperiodic motion on quasi-conic sections. These equations can be solved only numerically but their right-hand sides contain many oscillating terms and so it is very difficult to obtain their solutions over long time intervals with necessary precision. To simplify calculations and to analyze the behavior of orbital parameters over long time intervals we replace the perturbing functions by their secular parts and obtain a system of the evolutionary equations composed by 28 non-autonomous linear differential equations of the first order. Choosing some realistic laws of mass variations and physics parameters corresponding to the exoplanetary system TRAPPIST, we found numerical solutions of the evolutionary equations. All the relevant symbolic and numeric calculations are performed with the aid of the computer algebra system Wolfram Mathematica.

Simulation-Based Optimisation Model as an Element of a Digital Twin Concept for Supply Chain Inventory Control

Bożena Mielczarek, Maja Gora and Anna Dobrowolska

Abstract. Supply chain management is a critical success factor for many manufacturing companies. During the pandemic period, the problem of meeting delivery on time according to customer needs has intensified in many companies around the world. Companies would like to keep inventories at a level that ensures smooth order fulfillment while minimising their own costs. Deter-mining the optimal parameters is, however, a major challenge for Supply Chain inventory policy (SC). Combining simulation methods with optimisation techniques offers a methodology for obtaining an acceptable solution and, at the same time, provides a high degree of flexibility in the formulation of assumptions and the possibility of improving the decision-making process with respect to risk management. In this paper we present a simulation-based optimisation model to improve the quality of inventory management decisions in SC design and planning. Finally, we refer to the benefits of implementing the model in the concept of digital twins.