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# Computational Science – ICCS 2021

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# Preface

Welcome to the proceedings of the 21st annual International Conference on Computational Science (ICCS 2021 - <https://www.iccs-meeting.org/iccs2021/>).

In preparing this edition, we had high hopes that the ongoing COVID-19 pandemic would fade away and allow us to meet this June in the beautiful city of Kraków, Poland. Unfortunately, this 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 was 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 an increasing number of attendees and higher quality papers, and this year is not an exception, with over 350 registered participants. The proceedings 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 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 models, algorithms, and tools drive new science through efficient application in physical systems, computational and systems biology, environmental systems, finance, and other areas.

ICCS is well known for its excellent lineup of keynote speakers. The keynotes for 2021 were given by

- **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 were accepted (44%). A high acceptance rate in the thematic tracks is explained by the nature of these tracks, where 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

Maciej Paszynski  
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# Contents – Part IV

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

The Methods and Approaches of Explainable Artificial Intelligence. . . . .	3
<i>Mateusz Szczepański, Michał Choraś, Marek Pawlicki, and Aleksandra Pawlicka</i>	
Fake or Real? The Novel Approach to Detecting Online Disinformation Based on Multi ML Classifiers . . . . .	18
<i>Martyna Tarczewska, Anna Marciniak, and Agata Gielczyk</i>	
Transformer Based Models in Fake News Detection . . . . .	28
<i>Sebastian Kula, Rafał Kozik, Michał Choraś, and Michał Woźniak</i>	
Towards Model-Agnostic Ensemble Explanations . . . . .	39
<i>Szymon Bobek, Paweł Bałaga, and Grzegorz J. Nalepa</i>	

## Computational Methods in Smart Agriculture

Bluetooth Low Energy Livestock Positioning for Smart Farming Applications . . . . .	55
<i>Maciej Nikodem</i>	
Monitoring the Uniformity of Fish Feeding Based on Image Feature Analysis. . . . .	68
<i>Piotr Lech, Krzysztof Okarma, Agata Korzelecka-Orkisz, Adam Tański, and Krzysztof Formicki</i>	
A New Multi-objective Approach to Optimize Irrigation Using a Crop Simulation Model and Weather History . . . . .	75
<i>Mikhail Gasanov, Daniil Merkulov, Artyom Nikitin, Sergey Matveev, Nikita Stasenko, Anna Petrovskaia, Mariia Pukalchik, and Ivan Oseledets</i>	

## Computational Optimization, Modelling and Simulation

Expedited Trust-Region-Based Design Closure of Antennas by Variable-Resolution EM Simulations. . . . .	91
<i>Slawomir Koziel, Anna Pietrenko-Dabrowska, and Leifur Leifsson</i>	
Optimum Design of Tuned Mass Dampers for Adjacent Structures via Flower Pollination Algorithm . . . . .	105
<i>Sinan Melih Nigdeli, Gebrail Bekdas, and Xin-She Yang</i>	

On Fast Multi-objective Optimization of Antenna Structures Using Pareto Front Triangulation and Inverse Surrogates. . . . .	116
<i>Anna Pietrenko-Dabrowska, Slawomir Koziel, and Leifur Leifsson</i>	
Optimizations of a Generic Holographic Projection Model for GPU's . . . . .	131
<i>Mark Voschezang and Martin Fransen</i>	
Similarity and Conformity Graphs in Lighting Optimization and Assessment . . . . .	145
<i>Artur Basiura, Adam Sędziwy, and Konrad Komnata</i>	
Pruned Simulation-Based Optimal Sailboat Path Search Using Micro HPC Systems . . . . .	158
<i>Roman Dębski and Bartłomiej Sniezynski</i>	
Two Stage Approach to Optimize Electricity Contract Capacity Problem for Commercial Customers. . . . .	173
<i>Rafik Naikha, Tomasz Ząbkowski, and Krzysztof Gajowniczek</i>	
Improved Design Closure of Compact Microwave Circuits by Means of Performance Requirement Adaptation . . . . .	185
<i>Slawomir Koziel, Anna Pietrenko-Dabrowska, and Leifur Leifsson</i>	
Graph-Grammar Based Longest-Edge Refinement Algorithm for Three-Dimensional Optimally $p$ Refined Meshes with Tetrahedral Elements . . . . .	200
<i>Albert Mosialek, Andrzej Szaflarski, Rafal Pych, Marek Kisiel-Dorohinicki, Maciej Paszyński, and Anna Paszyńska</i>	
Elitism in Multiobjective Hierarchical Strategy . . . . .	214
<i>Michał Idzik, Radosław Łazarz, and Aleksander Byrski</i>	
Modelling and Forecasting Based on Recurrent Pseudoinverse Matrices. . . . .	229
<i>Christos K. Filelis-Papadopoulos, Panagiotis E. Kyziropoulos, John P. Morrison, and Philip O'Reilly</i>	
Semi-analytical Monte Carlo Optimisation Method Applied to the Inverse Poisson Problem . . . . .	243
<i>Slawomir Milewski</i>	
Modeling the Contribution of Agriculture Towards Soil Nitrogen Surplus in Iowa . . . . .	257
<i>Vishal Raul, Yen-Chen Liu, Leifur Leifsson, and Amy Kaleita</i>	
An Attempt to Replace System Dynamics with Discrete Rate Modeling in Demographic Simulations. . . . .	269
<i>Jacek Zabawa and Bożena Mielczarek</i>	

New On-line Algorithms for Modelling, Identification and Simulation of Dynamic Systems Using Modulating Functions and Non-asymptotic State Estimators: Case Study for a Chosen Physical Process . . . . .	284
<i>Witold Byrski, Michał Drapała, and Jędrzej Byrski</i>	
Iterative Global Sensitivity Analysis Algorithm with Neural Network Surrogate Modeling . . . . .	298
<i>Yen-Chen Liu, Jethro Nagawkar, Leifur Leifsson, Sławomir Koziel, and Anna Pietrenko-Dabrowska</i>	
Forecasting Electricity Prices: Autoregressive Hybrid Nearest Neighbors (ARHNN) Method . . . . .	312
<i>Weronika Nitka, Tomasz Serafin, and Dimitrios Sotiros</i>	
Data-Driven Methods for Weather Forecast . . . . .	326
<i>Elias David Nino-Ruiz and Felipe J. Acevedo García</i>	
Generic Case of Leap-Frog Algorithm for Optimal Knots Selection in Fitting Reduced Data . . . . .	337
<i>Ryszard Kozera, Lyle Noakes, and Artur Wiliński</i>	
Intelligent Planning of Logistic Networks to Counteract Uncertainty Propagation . . . . .	351
<i>Przemysław Ignaciuk and Adam Dziomdziora</i>	
Modeling Traffic Forecasts with Probability in DWDM Optical Networks . . .	365
<i>Stanisław Kozdrowski, Piotr Sliwka, and Sławomir Sujecki</i>	
Endogenous Factors Affecting the Cost of Large-Scale Geo-Stationary Satellite Systems . . . . .	379
<i>Nazareen Sikkandar Basha, Leifur Leifsson, and Christina Bloebaum</i>	
Description of Electricity Consumption by Using Leading Hours Intra-day Model . . . . .	392
<i>Krzysztof Karpio, Piotr Łukasiewicz, Rafik Nafkha, and Arkadiusz Orłowski</i>	
The Problem of Tasks Scheduling with Due Dates in a Flexible Multi-machine Production Cell . . . . .	405
<i>Wojciech Bożejko, Piotr Nadybski, Paweł Rajba, and Mieczysław Wodecki</i>	
Discovering the Influence of Interruptions in Cycling Training: A Data Science Study . . . . .	420
<i>Alen Rajšp and Iztok Fister Jr.</i>	

Analysis of Complex Partial Seizure Using Non-linear Duffing Van der Pol Oscillator Model . . . . .	433
<i>Beata Szufliłowska and Przemysław Orłowski</i>	
<b>Computational Science in IoT and Smart Systems</b>	
A Review on Visual Programming for Distributed Computation in IoT . . . . .	443
<i>Margarida Silva, João Pedro Dias, André Restivo, and Hugo Sereno Ferreira</i>	
Data Preprocessing, Aggregation and Clustering for Agile Manufacturing Based on Automated Guided Vehicles . . . . .	458
<i>Rafał Cupek, Marek Drewniak, and Tomasz Steclik</i>	
Comparison of Speech Recognition and Natural Language Understanding Frameworks for Detection of Dangers with Smart Wearables . . . . .	471
<i>Dariusz Mrozek, Szymon Kwaśnicki, Vaidy Sunderam, Bożena Małysiak-Mrozek, Krzysztof Tokarz, and Stanisław Kozielski</i>	
A Decision Support System Based on Augmented Reality for the Safe Preparation of Chemotherapy Drugs . . . . .	485
<i>Sarah Ben Othman, Hayfa Zgaya, Michèle Vasseur, Bertrand Décaudin, Pascal Odou, and Slim Hammadi</i>	
Metagenomic Analysis at the Edge with Jetson Xavier NX . . . . .	500
<i>Piotr Grzesik and Dariusz Mrozek</i>	
Programming IoT-Spaces: A User-Survey on Home Automation Rules . . . . .	512
<i>Danny Soares, João Pedro Dias, André Restivo, and Hugo Sereno Ferreira</i>	
Application of the Ant Colony Algorithm for Routing in Next Generation Programmable Networks . . . . .	526
<i>Stanisław Kozdrowski, Magdalena Banaszek, Bartosz Jedrzejczak, Mateusz Żotkiewicz, and Zbigniew Kopertowski</i>	
Scalable Computing System with Two-Level Reconfiguration of Multi-channel Inter-Node Communication . . . . .	540
<i>Miroslaw Hajder, Piotr Hajder, Mateusz Liput, and Janusz Kolbusz</i>	
Real-Time Object Detection for Smart Connected Worker in 3D Printing . . . . .	554
<i>Shijie Bian, Tiancheng Lin, Chen Li, Yongwei Fu, Mengrui Jiang, Tongzi Wu, Xiyi Hang, and Bingbing Li</i>	
Object-Oriented Internet Cloud Interoperability . . . . .	568
<i>Mariusz Postół and Piotr Szymczak</i>	

Static and Dynamic Comparison of Pozyx and DecaWave UWB Indoor Localization Systems with Possible Improvements. . . . .	582
<i>Barbara Morawska, Piotr Lipiński, Krzysztof Lichy, Piotr Koch, and Marcin Leplawy</i>	
Challenges Associated with Sensors and Data Fusion for AGV-Driven Smart Manufacturing. . . . .	595
<i>Adam Ziebinski, Dariusz Mrozek, Rafal Cupek, Damian Grzechca, Marcin Fojcik, Marek Drewniak, Erik Kyrkjebø, Jerry Chun-Wei Lin, Knut Øvsthus, and Piotr Biernacki</i>	
Dynamic Pricing and Discounts by Means of Interactive Presentation Systems in Stationary Point of Sales . . . . .	609
<i>Marcin Lewicki, Tomasz Kajdanowicz, Piotr Bródka, and Janusz Sobecki</i>	
Profile-Driven Synthetic Trajectories Generation to Enhance Smart System Solutions . . . . .	623
<i>Radosław Klimek and Arkadiusz Olesek</i>	
Augmenting Automatic Clustering with Expert Knowledge and Explanations. . . . .	631
<i>Szymon Bobek and Grzegorz J. Nalepa</i>	
Renewable Energy-Aware Heuristic Algorithms for Edge Server Selection for Stream Data Processing . . . . .	639
<i>Tomasz Szydło and Chris Gniady</i>	
Dataset for Anomalies Detection in 3D Printing . . . . .	647
<i>Tomasz Szydło, Joanna Sendorek, Mateusz Windak, and Robert Brzoza-Wońch</i>	
Correction to: Computational Science – ICCS 2021. . . . .	C1
<i>Maciej Paszynski, Dieter Kranzlmüller, Valeria V. Krzhizhanovskaya, Jack J. Dongarra, and Peter M. A. Sloot</i>	
<b>Author Index . . . . .</b>	<b>655</b>