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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 II

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

Large-Scale Stabilized Multi-physics Earthquake Simulation for Digital Twin	3
<i>Ryota Kusakabe, Tsuyoshi Ichimura, Kohei Fujita, Muneo Hori, and Lalith Wijerathne</i>	
On the Design of Monte-Carlo Particle Coagulation Solver Interface: A CPU/GPU Super-Droplet Method Case Study with PySDM	16
<i>Piotr Bartman and Sylwester Arabas</i>	

Applications of Computational Methods in Artificial Intelligence and Machine Learning

A Deep Neural Network Based on Stacked Auto-encoder and Dataset Stratification in Indoor Location	33
<i>Jing Zhang and Ying Su</i>	
Recurrent Autoencoder with Sequence-Aware Encoding.	47
<i>Robert Susik</i>	
A Gist Information Guided Neural Network for Abstractive Summarization	58
<i>Yawei Kong, Lu Zhang, and Can Ma</i>	
Quality of Recommendations and Cold-Start Problem in Recommender Systems Based on Multi-clusters.	72
<i>Urszula Kuźelewska</i>	
Model of the Cold-Start Recommender System Based on the Petri-Markov Nets	87
<i>Mihail Chipchagov and Evgeniy Kublik</i>	
Text-Based Product Matching with Incomplete and Inconsistent Items Descriptions.	92
<i>Szymon Łukasik, Andrzej Michałowski, Piotr A. Kowalski, and Amir H. Gandomi</i>	
Unsupervised Text Style Transfer via an Enhanced Operation Pipeline	104
<i>Wanhui Qian, Jinzhu Yang, Fuqing Zhu, Yipeng Su, and Songlin Hu</i>	

Exemplar Guided Latent Pre-trained Dialogue Generation	118
<i>Miaojin Li, Peng Fu, Zheng Lin, Weiping Wang, and Wenyu Zang</i>	
Monte Carlo Winning Tickets.	133
<i>Rafał Grzeszczuk and Marcin Kurdziel</i>	
Interpreting Neural Networks Prediction for a Single Instance via Random Forest Feature Contributions.	140
<i>Anna Palczewska and Urszula Markowska-Kaczmar</i>	
A Higher-Order Adaptive Network Model to Simulate Development of and Recovery from PTSD	154
<i>Laila van Ments and Jan Treur</i>	
Trojan Traffic Detection Based on Meta-learning	167
<i>Zijian Jia, Yepeng Yao, Qiuyun Wang, Xuren Wang, Baoxu Liu, and Zhengwei Jiang</i>	
Grasp the Key: Towards Fast and Accurate Host-Based Intrusion Detection in Data Centers.	181
<i>Mengtian Gu, Biyu Zhou, Fengyang Du, Xuehai Tang, Wang Wang, Liangjun Zang, Jizhong Han, and Songlin Hu</i>	
MGEL: A Robust Malware Encrypted Traffic Detection Method Based on Ensemble Learning with Multi-grained Features	195
<i>Juncheng Guo, Yafei Sang, Peng Chang, Xiaolin Xu, and Yongzheng Zhang</i>	
TS-Bert: Time Series Anomaly Detection via Pre-training Model Bert.	209
<i>Weixia Dang, Biyu Zhou, Lingwei Wei, Weigang Zhang, Ziang Yang, and Songlin Hu</i>	
Relation Order Histograms as a Network Embedding Tool.	224
<i>Radosław Łazarz and Michał Idzik</i>	
Desensitization Due to Overstimulation: A Second-Order Adaptive Network Model.	238
<i>Alex Korthouwer, David Noordberg, and Jan Treur</i>	
A Modified Deep Q-Network Algorithm Applied to the Evacuation Problem	250
<i>Marcin Skulimowski</i>	
Human-Like Storyteller: A Hierarchical Network with Gated Memory for Visual Storytelling	257
<i>Lu Zhang, Yawei Kong, Fang Fang, Cong Cao, Yanan Cao, Yanbing Liu, and Can Ma</i>	

Discriminative Bayesian Filtering for the Semi-supervised Augmentation of Sequential Observation Data.	271
<i>Michael C. Burkhardt</i>	
TSAX is Trending.	284
<i>Muhammad Marwan Muhammad Fuad</i>	
MultiEmo: Multilingual, Multilevel, Multidomain Sentiment Analysis Corpus of Consumer Reviews.	297
<i>Jan Kocoń, Piotr Miłkowski, and Kamil Kanclerz</i>	
Artificial Intelligence and High-Performance Computing for Advanced Simulations	
Outlier Removal for Isogeometric Spectral Approximation with the Optimally-Blended Quadratures	315
<i>Quanling Deng and Victor M. Calo</i>	
Socio-cognitive Evolution Strategies	329
<i>Aleksandra Urbańczyk, Bartosz Nowak, Patryk Orzechowski, Jason H. Moore, Marek Kisiel-Dorohinicki, and Aleksander Byrski</i>	
Effective Solution of Ill-Posed Inverse Problems with Stabilized Forward Solver.	343
<i>Marcin Łoś, Robert Schaefer, and Maciej Smółka</i>	
Supermodeling - A Meta-procedure for Data Assimilation and Parameters Estimation	358
<i>Leszek Siwik, Marcin Łoś, and Witold Dzwiniel</i>	
AI-Accelerated CFD Simulation Based on OpenFOAM and CPU/GPU Computing	373
<i>Krzysztof Rojek, Roman Wyrzykowski, and Pawel Gepner</i>	
An Application of a Pseudo-Parabolic Modeling to Texture Image Recognition	386
<i>Joao B. Florindo and Eduardo Abreu</i>	
A Study on a Feedforward Neural Network to Solve Partial Differential Equations in Hyperbolic-Transport Problems	398
<i>Eduardo Abreu and Joao B. Florindo</i>	
Agent-Based Modeling of Social Phenomena for High Performance Distributed Simulations	412
<i>Mateusz Paciorek and Wojciech Turek</i>	
Automated Method for Evaluating Neural Network's Attention Focus	426
<i>Tomasz Szandala and Henryk Maciejewski</i>	

Machine Learning Control Design for Elastic Composite Materials	437
<i>Sebastián Ossandón, Mauricio Barrientos, and Camilo Reyes</i>	
Optimize Memory Usage in Vector Particle-In-Cell (VPIC) to Break the 10 Trillion Particle Barrier in Plasma Simulations	452
<i>Nigel Tan, Robert Bird, Guangye Chen, and Michela Taufer</i>	
Deep Learning for Prediction of Complex Geology Ahead of Drilling	466
<i>Kristian Fossum, Sergey Alyaev, Jan Tveranger, and Ahmed Elsheikh</i>	
Biomedical and Bioinformatics Challenges for Computer Science	
Controlling Costs in Feature Selection: Information Theoretic Approach	483
<i>Paweł Teisseyre and Tomasz Klonecki</i>	
How Fast Vaccination Can Control the COVID-19 Pandemic in Brazil?	497
<i>Rafael Sachetto Oliveira, Carolina Ribeiro Xavier, Vinícius da Fonseca Vieira, Bernardo Martins Rocha, Ruy Freitas Reis, Bárbara de Melo Quintela, Marcelo Lobosco, and Rodrigo Weber dos Santos</i>	
Uncertainty Quantification of Tissue Damage Due to Blood Velocity in Hyperthermia Cancer Treatments.	511
<i>Bruno Rocha Guedes, Marcelo Lobosco, Rodrigo Weber dos Santos, and Ruy Freitas Reis</i>	
EEG-Based Emotion Recognition – Evaluation Methodology Revisited	525
<i>Sławomir Opalka, Bartłomiej Stasiak, Agnieszka Wosiak, Aleksandra Dura, and Adam Wojciechowski</i>	
Modeling the Electromechanics of a Single Cardiac Myocyte	540
<i>Anna Luisa de Aguiar Bergo Coelho, Ricardo Silva Campos, João Gabriel Rocha Silva, Carolina Ribeiro Xavier, and Rodrigo Weber dos Santos</i>	
Towards Mimetic Membrane Systems in Molecular Dynamics: Characteristics of <i>E. Coli</i> Membrane System	551
<i>Mateusz Rzycki, Sebastian Kraszewski, and Dominik Drabik</i>	
PathMEX: Pathway-Based Mutual Exclusivity for Discovering Rare Cancer Driver Mutations.	564
<i>Yahya Bokhari and Tomasz Arodz</i>	
Serverless Nanopore Basecalling with AWS Lambda.	578
<i>Piotr Grzesik and Dariusz Mrozek</i>	

A Software Pipeline Based on Sentiment Analysis to Analyze Narrative Medicine Texts	587
<i>Ileana Scarpino, Chiara Zucco, and Mario Cannataro</i>	
Author Index	595