Journal of Computational Science 81 (2024) 102379

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Computation at the Cutting Edge of Science

1. Introduction

The area of computational science [1] is developing at the intersection of computer science, information technologies, and mathematical modeling. Being an interdisciplinary area by its nature, it incorporates and integrates a multitude of diverse methodologies, concepts, and tools. The list of computational science applications spans from traditional application scenarios in natural sciences to emerging and relatively new fields like computational medicine, social sciences, and humanities. Moreover, computational science stimulates the development of novel application areas, and it may propose new interdisciplinary research at the intersection of diverse application areas and innovative modes of computational thinking.

Computational science plays multiple crucial roles in today's scientific agenda. Firstly, it continues to support advancements in diverse domains by leveraging computational models to gain new insights into natural and social phenomena across different scales. Secondly, it has evolved into a robust and independent field with its own conceptual and methodological framework. Computational science integrates two primary scientific approaches centered around the notion of a computational experiment. This experiment is designed and constructed based on domain knowledge and problem definition, leading to deductive or knowledge-based inferences of models and computational solutions. In addition, data-driven approaches and methods can be employed for inductive (empirical) inference. The combination of these approaches, coupled with the availability of computational resources, empowers computational science to innovate and adapt general-purpose concepts and technologies. Initially, the research field originated at the intersection of mathematical modeling algorithms (including numerical simulation) and computationally intensive solutions (such as high-performance, distributed, or hybrid computing). However, it has now emerged as an independent discipline, with a heightened focus on scalability, openness, and reproducibility [2].

Furthermore, computational science has embraced the latest advancements in information and computer science technologies, offering novel solutions to existing challenges within the field. One notable development is the vast amount of data that is now being collected through observations, measurements, or from previous modeling and simulations. This data serves as a valuable resource for scientific discovery, leading some scholars to consider it as a new paradigm known as data-intensive scientific discovery, often referred to as the fourth scientific paradigm [3]. These approaches, accompanied by the foundational concepts of Big Data, have found their place in the realm of computational science [4].

Lately, there has been a significant surge of interest within the scientific community towards artificial intelligence and machine learning methods, which can be seen as another extension of computational science. These methods have the potential to fulfill several roles within the computational science domain. Firstly, they can aid in managing complex models. Secondly, they can serve as substitutes for computationally intensive models. Additionally, they can facilitate the exploration and interpolation of model parameters and data. Lastly, they can contribute to predicting various characteristics of models, including performance, uncertainty, sensitivity, and more [5–8].

Computational science plays a crucial role in supporting the development of new areas and directions in science. One notable example is simulation-based engineering science [9], which utilizes computational simulations to advance engineering practices. Another important application area is simulation-based decision-making [10], where computational models aid in making informed decisions. Computational science also finds value in multidisciplinary studies, where the integration of multiple models provides a comprehensive understanding of complex systems and phenomena. The concept of system-level science [11], for instance, emphasizes a holistic description of a system to enable analysis and computational experiments with diverse objectives using a unified solution.

Considering all these aspects, computational science can be regarded as a driving force for scientific and technological advancements, contributing to a better future. It provides novel tools for research and development in crucial areas, identifies and addresses new problems with innovative methods, and fosters entirely new approaches to scientific evolution. In line with this vision, we are delighted to introduce a special issue inspired by the theme "**Computation at the Cutting Edge of Science**," which stems from the International Conference on Computational Science (ICCS) 2023. This special issue aims to tackle the current challenges in the quest for sustainable development.

Since its inception in 2001, ICCS has been a gathering point for researchers and scientists working in various application areas and fundamental computer science disciplines. The conference showcases the pioneering use of computational methods in fields such as physics, chemistry, life sciences, engineering, as well as arts and humanities. ICCS has been hosted by different institutions and cities across 13 countries, including Australia, Czechia, China, Iceland, Poland, Portugal, Russia, the Netherlands, Singapore, Spain, Switzerland, the UK, and the USA. Throughout its history, ICCS has always been focused on recent advancements in computational science.

Analyzing the evolution of ICCS topics [12,13] reveals a significant concentration of works presented at the conference in key sub-areas of computational science, such as modeling and simulation, high-performance and distributed computing, and numerical methods.

https://doi.org/10.1016/j.jocs.2024.102379

Available online 25 June 2024

Moreover, ICCS remains responsive to emerging technologies and approaches, such as the development of GPGPU or IPv6 technologies, as evidenced by the increasing number of publications in these respective areas. The dynamic of topics over the recent 23 years (see Fig. 1) shows a constant interest of the community in "modeling and simulation", and "algorithms and data structures", which form the core of computational science methodology. At the same time, a significant growth of interest in AI and machine learning is seen in the last 7 years (see also Table 1). More details on the topic analysis can be found in [13].

The ICCS society continues to attract renowned scientists as well as young researchers. Three years ago, we had the pleasure of announcing a special issue of the Journal of Computational Science. This issue featured 12 selected papers authored by leading scientists in the field, who had served as keynote speakers throughout the 20-year history of ICCS, along with their colleagues. These papers provided insights into the vision, recent advancements, challenges, and solutions in various sub-areas [14].

The evolution of ICCS title themes reflects a significant interest in addressing global challenges. Recent themes of ICCS have focused on open problems and broader, more diverse applications of computational science, illustrating the expanding influence of the field. Examples of such themes include "Computation at the Frontiers of Science" (ICCS 2013), "Computational Science at the Gates of Nature" (ICCS 2015), "The Art of Computational Science. Bridging Gaps – Forming Alloys" (ICCS 2017), "Computational Science in the Interconnected World" (ICCS 2019), "Computational Science for a Better Future" (ICCS 2021), "The Computational Planet" (ICCS 2022), and, of course, "Computation at the Cutting Edge of Science" (ICCS 2023). These themes highlight the integral role of computational science in addressing modern challenges across various domains, including the natural sciences, economics, and social sciences.

The adaptability of ICCS is also reflected in its thematic tracks and workshops, which focus on the most important topics in the field. ICCS has proudly hosted thematic tracks such as "Multiscale Modelling and Simulation," "Computational Optimization, Modelling and Simulation," "Data-Driven Computational Sciences," "Agent-Based Simulations, Adaptive Algorithms and Solvers," "Biomedical and Bioinformatics Challenges," "Teaching Computational Science," and many others, providing a platform for in-depth discussions and knowledge exchange.

Table 1
Top 20 second-level disciplines for 23 years and in 2023 [13].

Top 20 in 23 years	Average rank	Top 20 in 2023	Rank
Algorithm	2.83	Machine learning	1
Numerical analysis	4.13	Deep learning	2
Machine learning	4.61	Mathematical modelling	3
Mathematical model	5.83	Artificial intelligence	4
Computer simulation	7.96	Algorithm	5
Data & information visualization	8.35	Numerical analysis	6
Parallel computing	10.00	Computational sociology	7
Computational sociology	10.78	ABM	8
Mathematical optimization	10.82	Data & information visualization	9
Genetic algorithm	11.26	Data mining	10
GPGPU	11.52	Stochastic simulation	11
Stochastic simulation	11.95	Mathematical optimization	12
ABM	13.48	Cross-validation	13
Data mining	13.96	Computer simulation	14
Distributed computing	14.57	Scientific modelling	15
Computational science	15.70	Genetic algorithm	16
Data structure	17.96	Reinforcement learning	17
Artificial intelligence	18.00	Computational chemistry	18
Deep learning	20.04	GPGPU	19
Database	20.52	Natural language processing	20

2. Overview of the virtual special issue

We are glad to present this virtual special issue of the Journal of Computational Science with selected extended papers from ICCS 2023. This issue continues the sequence of annual collections of key ICCS publications [15,16]. The issue contains extended papers demonstrating the various topics relevant to the ICCS society. These topics were selected from 282 papers published in the ICCS 2023 conference proceedings in Vol. 14073–14077 by Lecture Notes in Computer Science [17], which were selected from over 531 submissions.

As usual, many ICCS papers report on **numerical methods** development, improvement, and implementation, as they form the core of the computational science area. Kolar-Požun et al. [18] present an original study on Radial Basis Function-generated Finite Difference (RBF-FD) method for partial differential equation solving affected by stencil size parameter. Rot et al. [19] investigate computational cost reduction in meshless approximation with original approach to coverage of the considered domain with scattered nodes. Sikora et al. [20] presented a

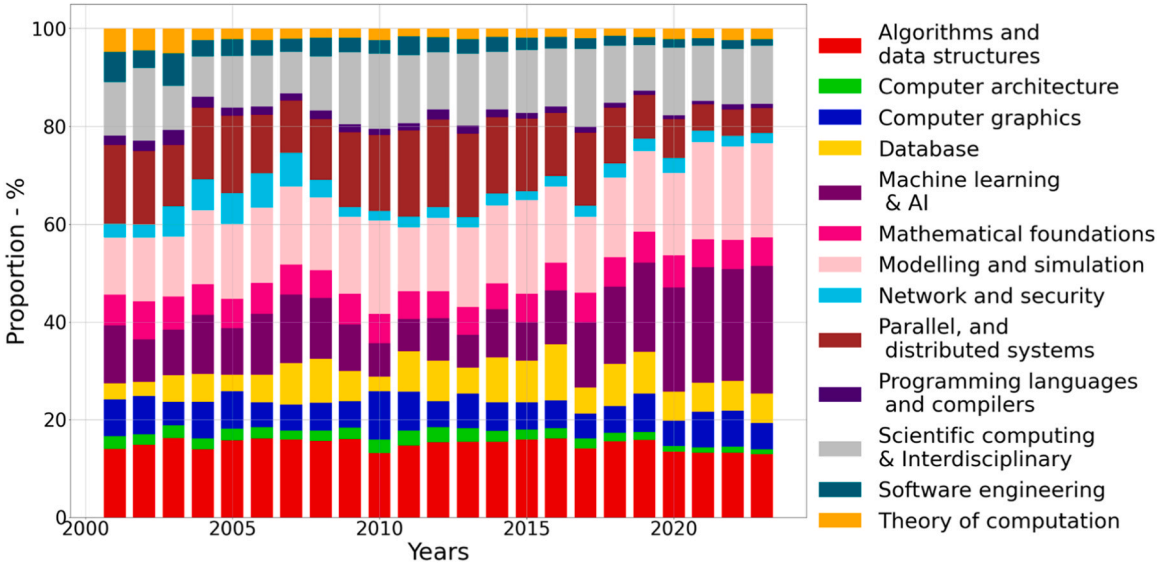

Fig. 1. - Percentage of high-level topics in ICCS papers [13].

comparative study of regular and variational physics-informed neural networks in application to high-order and continuity finite element method. Mahadevan et al. [21] proposed a new domain decomposition method for computing multivariate functional approximations with B-spline to reduce the total work per task.

Complex systems usually attract significant interest in computational science community. Complex networks, agent-based modeling, and other applications are widely adopted here. Kwak et al. [22] investigate crowd dynamics with a specific focus on pedestrian motion and interaction to provide a sufficient basis for modelling interaction with spreading information, disease, or substances. Aref and Mostajabdaveh [23] studied modularity-based algorithms for community detection with analysis of limitation in popular algorithms and approaches. Blanco et al. [24] investigate possible reconstruction of brain connectivity network and functional properties from electroencephalography and functional near-infrared spectroscopy. Olsen et al. [25] propose a general approach to train a machine learning model in successfully predicting the outcome of an agent-based model using data generated only from a small subset of parameter value combinations. Díaz et al. [26] introduce an Intelligent Transportation System, ITS4T-sunamis, that combines different technologies to help emergency management agencies provide safe routes to their emergency vehicles.

An important part of computational science is **algorithms and software** development, including software for high-performance and distributed computing and data-driven algorithms (recently enriched with many works based on advances in machine learning and AI). This part includes original algorithms introduced within the computational science area. For example, Jastrząb et al. [27] is studying inference and evaluation of nondeterministic finite automata for learning formal grammar rules.

An important sub-area recently gained significant progress is machine learning algorithms and solutions within computational science. Pereira et al. [28] propose original Siamese autoencoder-based approach for missing data imputation, showing improvement comparing to popular stat-of-the-art solutions. Szarmach and Czarnowski [29] proposed multi-class classification based approach for anomalies and damage detection in information processed in automatic identification systems applied in marine equipment identification. Freitas et al. [30] developed machine learning models able to successfully execute complex aircraft maneuvers; these models were trained on maneuvers from human pilots and in some instances exhibited superior performance to the pilots themselves. Pogrebnoy et al. [31] propose a new method and tool (RuMedSpellchecker) for efficiently correcting spelling errors in Russian medical texts.

While the directions mentioned earlier change the area itself, a significant role of computational science is the **application** of the developed methods to various problem domains. Here, computational science provides new solutions to tackle the problems and build a better future. Łoś et al. [32] presented a numerical experimental study on effectiveness of hail cannoning for preventing cloud formation and local weather control. Kishi et al. [33] demonstrated an experimental study on simulation of virus-laden droplet transportation from the lung of infected patient to exposed one depending on neck angle and particle size for better understanding of pulmonary diseases spreading. Vidal et al. [34] presents a study on air quality and green infrastructure in the city of Barcelona using coupled modelling approach based on WRF-Chem and BEP/BEM models and possible extension with machine learning.

We believe that this collection of papers represents the cutting-edge advancements and dynamics within the field of computational science. These papers not only capture the current trends in the field but also address emerging problems that hold the potential to shape a better future. We are confident that these papers will be of great interest to the broader scientific community, including researchers and professionals in the field of computational science, as well as various application domains.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We thank the authors of the selected papers for their valuable contributions, the reviewers of this special issue for their in-depth reviews and constructive comments, the ICCS program committee members, and track organizers for their diligent work ensuring the high standard of accepted ICCS papers. As always, we also thank Springer for publishing the conference proceedings and Elsevier for their continuous support and inspiration during the preparation and publishing of this virtual special issue.

References

[1] P. Sloot, P. Coveney, J. Dongarra, Preface, J. Comput. Sci. 1 (2010) 3–4, https://doi.org/10.1016/j.jocs.2010.04.003.
[2] L.A. Barba, Praxis of reproducible computational science, Comput. Sci. Eng. 21 (2019) 73–78, https://doi.org/10.1109/MCSE.2018.2881905.
[3] T. Hey, S. Tansley, and K. Tolle, eds., The Fourth Paradigm: Data-Intensive Scientific Discovery, Microsoft Research, 2009.
[4] M.D. Assunção, R.N. Calheiros, S. Bianchi, M.A.S. Netto, R. Buyya, Big Data computing and clouds: trends and future directions, J. Parallel Distrib. Comput. 79–80 (2015) 3–15, https://doi.org/10.1016/j.jpdc.2014.08.003.
[5] S. Koziel, D.E. Ciaurri, L. Leifsson, Surrogate-based methods, : Comput. Optim. Methods Algorithms (2011) 33–59, https://doi.org/10.1007/978-3-642-20859-1_3.
[6] D. Lim, Yaochu Jin, Yew-Soon Ong, B. Sendhoff, Generalizing surrogate-assisted evolutionary computation, IEEE Trans. Evol. Comput. 14 (2010) 329–355, https://doi.org/10.1109/TEVC.2009.2027359.
[7] A.A. Funkner, S.V. Kovalchuk, A.N. Yakovlev, Surrogate-assisted performance prediction for data-driven knowledge discovery algorithms: Application to evolutionary modeling of clinical pathways, J. Comput. Sci. 59 (2022) 101562, https://doi.org/10.1016/j.jocs.2022.101562.
[8] D. Ye, P. Zun, V. Krzhizhanovskaya, A.G. Hoekstra, Uncertainty quantification of a three-dimensional in-stent restenosis model with surrogate modelling, J. R. Soc. Interface 19 (2022), https://doi.org/10.1098/rsif.2021.0864.
[9] S.C. Glotzer, International Assessment of Research and Development in Simulation-Based Engineering and Science, IMPERIAL COLLEGE PRESS, 2011. doi:10.1142/p777.
[10] A.R. Tilman, V.V. Vasconcelos, E. Akcay, J.B. Plotkin, The evolution of forecasting for decision making in dynamic environments, ArXiv Prepr. (2021) arXiv:2108.00047.
[11] I. Foster, C. Kesselman, Scaling System-Level Science: Scientific Exploration and IT Implications, Computer 39 (2006) 31–39, https://doi.org/10.1109/MC.2006.397.
[12] T.M. Abuhay, S.V. Kovalchuk, K. Bochenina, G.-K. Mbogo, A.A. Visheratin, G. Kampis, V.V. Krzhizhanovskaya, M.H. Lees, Analysis of publication activity of computational science society in 2001-2017 using topic modeling and graph theory, J. Comput. Sci. (2018), https://doi.org/10.1016/j.jocs.2018.04.004.
[13] L. Luo, S. Kovalchuk, V. Krzhizhanovskaya, M. Paszynski, C. de Mulatier, J. Dongarra, P.M.A. Sloot, Trends in Computational Science: Natural Language Processing and Network Analysis of 23 Years of ICCS Publications, Lect. Notes Comput. Sci. 14833 (2024) 19–33, https://doi.org/10.1007/978-3-031-63751-3_2.
[14] S.V. Kovalchuk, V.V. Krzhizhanovskaya, P.M.A. Sloot 20 years of computational science // Journal of Computational Science, 2020, Vol. 46, pp. 101187. doi: 10.1016/j.jocs.2020.101187.
[15] S.V. Kovalchuk, V.V. Krzhizhanovskaya, M. Paszyński, D. Kranzlmüller, J. Dongarra, P.M.A. Sloot, Computational science for a better future, J. Comput. Sci. 62 (2022) 101745, https://doi.org/10.1016/j.jocs.2022.101745.
[16] S.V. Kovalchuk, C. de Mulatier, D. Groen, M. Paszyński, V.V. Krzhizhanovskaya, J. Dongarra, P.M.A. Sloot, The computational planet, J. Comput. Sci. 72 (2023) 102102, https://doi.org/10.1016/j.jocs.2023.102102.
[17] J. Mikyška, C. de Mulatier, M. Paszynski, V.V. Krzhizhanovskaya, J. Dongarra, P.M. A. Sloot, Computational Science – ICCS 2023. Preface (v–vi), Lect. Notes Comput. Sci. 14073 (2023), https://doi.org/10.1007/978-3-031-35995-8.
[18] A. Kolar-Požun, M. Jančič, M. Rot, G. Kosec, Some observations regarding the RBF-FD approximation accuracy dependence on stencil size, in: Journal of Computational Science, 79, Elsevier BV,, Jul. 2024, https://doi.org/10.1016/j.jocs.2024.102284.
[19] M. Rot, M. Jančič, G. Kosec, Spatially dependent node regularity in meshless approximation of partial differential equations, in: Journal of Computational Science, 79, Elsevier BV,, Jul. 2024, https://doi.org/10.1016/j.jocs.2024.102306.
[20] M. Sikora, P. Krukowski, A. Paszyńska, M. Paszyński, Comparison of Physics Informed Neural Networks and Finite Element Method Solvers for advection-dominated diffusion problems, in: Journal of Computational Science, 81, Elsevier BV,, Sep. 2024, https://doi.org/10.1016/j.jocs.2024.102340.

[21] V. Mahadevan, D. Lenz, I. Grindeanu, T. Peterka, Accelerating multivariate functional approximation computation with domain decomposition techniques, in: Journal of Computational Science, 78, Elsevier BV,, Jun. 2024, https://doi.org/10.1016/j.jocs.2024.102268.
[22] J. Kwak, M. Lees, W. Cai, Characterizing pedestrian contact interaction trajectories to understand spreading risk in human crowds, J. Comput. Sci. (2024) in press.
[23] S. Aref, M. Mostajabdaveh, Analyzing modularity maximization in approximation, heuristic, and graph neural network algorithms for community detection, in: Journal of Computational Science, 78, Elsevier BV,, Jun. 2024, https://doi.org/10.1016/j.jocs.2024.102283.
[24] R. Blanco, C. Koba, A. Crimi, Investigating the interaction between EEG and fNIRS: a multimodal network analysis of brain connectivity, J. Comput. Sci. (2024) under review.
[25] M. Olsen, M.S. Raunak, D.R. Kuhn, On Using Covering Arrays and Machine Learning to Explore Agent-Based Model Parameters, J. Comput. Sci. (2024) in press.
[26] G. Diaz-Descalzo, H. Macià, E. Brazalez, J. Boubeta-Puig, M.C. Ruiz, V. Valero, ITS4Tsunamis: an intelligent transportation system for tsunami emergencies, J. Comput. Sci. (2024) under review.
[27] T. Jastrzab, F. Lardeux, E. Monfroy, Robust models to infer flexible nondeterministic finite automata, in: Journal of Computational Science, 79, Elsevier BV,, Jul. 2024, https://doi.org/10.1016/j.jocs.2024.102309.
[28] R.C. Pereira, P.H. Abreu, P.P. Rodrigues, Siamese Autoencoder Architecture for the Imputation of Data Missing Not at Random, in: Journal of Computational Science, 78, Elsevier BV,, Jun. 2024, https://doi.org/10.1016/j.jocs.2024.102269.
[29] M. Szarmach, I. Czarnowski, A framework for damage detection in AIS data based on clustering and multi-label classification, in: Journal of Computational Science, 76, Elsevier BV,, Mar. 2024, https://doi.org/10.1016/j.jocs.2024.102218.
[30] H. Freitas, R. Camacho, D.C. Silva, Imitation Learning for Aerobatic Maneuvering in Fixed-Wing Aircraft, J. Comput. Sci. (2024) in press.
[31] D. Pogrebnoy, A. Funkner, S. Kovalchuck, RuMedSpellchecker: new approach for advanced spelling error correction in Russian electronic health records, J. Comput. Sci. (2024) under review.
[32] M. Łoś, et al., Shock waves generators: From prevention of hail storms to reduction of the smog in urban areas — experimental verification and numerical simulations, in: Journal of Computational Science, 77, Elsevier BV,, Apr. 2024, https://doi.org/10.1016/j.jocs.2024.102238.
[33] S. Kishi, M. Yamakawa, A. Takii, S. Asao, S. Takeuchi, M. Kim, Impact of neck angle variation on particle and virus-laden droplet transport from lung to lung using eighth-generation airway model, in: Journal of Computational Science, 75, Elsevier BV,, Jan. 2024, https://doi.org/10.1016/j.jocs.2023.102202.
[34] V. Vidal, A. Cortés, A. Badia, G. Villalba, Modeling air quality at urban scale in the city of Barcelona: a matter of green resolution, in: Journal of Computational Science, 79, Elsevier BV,, Jul. 2024, https://doi.org/10.1016/j.jocs.2024.102289.

Sergey V. Kovalchuk[a], Clélia de Mulatier[b], Valeria V. Krzhizhanovskaya[b], Jiří Mikyška[c], Maciej Paszyński[d], Jack Dongarra[e], Peter M.A. Sloot[b]
[a] *International Conference on Computational Science*
[b] *University of Amsterdam, Amsterdam, the Netherlands*
[c] *Czech Technical University in Prague, Prague, Czech Republic*
[d] *AGH University of Krakow, Krakow, Poland*
[e] *University of Tennessee, Knoxville, USA*