Computational science

Guiding the way towards a sustainable society

Kovalchuk, Sergey V.; de Mulatier, Clélia; Krzhizhanovskaya, Valeria V.; Franco, Leonardo; Paszyński, Maciej; Dongarra, Jack; Sloot, Peter M.A.

DOI
10.1016/j.jocs.2025.102663

Publication date
2025

Document Version
Final published version

Published in
Journal of Computational Science

Journal of Computational Science 90 (2025) 102663

Contents lists available at ScienceDirect

Journal of Computational Science

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

Computational science: Guiding the way towards a sustainable society

1. Introduction

Computational science [1] represents a dynamic and interdisciplinary domain situated at the intersection of computer science, mathematical modeling, and information technology. Historically, it has served as a catalyst for scientific advancement across diverse fields – from engineering to biomedicine – by leveraging computational experiments to generate new insights into natural and social phenomena. Today, this discipline has evolved into an indispensable framework for addressing the defining challenge of our era: the urgent transition toward global sustainability. Computational science provides unprecedented capabilities to model, analyze, and optimize complex human-environment interactions through integrated approaches that combine deductive model-based reasoning with inductive data-driven methodologies [2,3].

The emergence of "computational sustainability science" marks a paradigm shift in tackling multifaceted challenges, including climate change mitigation, biodiversity conservation, and resource security [4,5]. This evolution reflects the maturation of computational science into an autonomous field characterized by rigorous methodological frameworks, a heightened emphasis on scalability and reproducibility [6], and the assimilation of transformative technologies. Crucially, the advent of data-intensive scientific discovery—recognized as the fourth scientific paradigm [2] – has empowered researchers to harness vast observational and simulated datasets. At the same time, artificial intelligence and machine learning now fulfill multifaceted roles: managing intricate systems, substituting computationally expensive models, and predicting system behaviors under uncertainty [7–10].

Contemporary advances demonstrate the pivotal capacity of computational science to navigate sustainability imperatives. In climate science, machine learning overcomes traditional limitations in Earth system modeling, with initiatives like ClimateLearn democratizing access to advanced forecasting tools [11]. At the same time, SmartSim's neural network architecture accelerates ocean simulations by orders of magnitude [12]. Renewable energy integration benefits from sophisticated optimization algorithms such as Grey Wolf Optimization and Particle Swarm Optimization, which enhance the placement and efficiency of solar and wind infrastructure [13,14]. Urban sustainability is similarly transformed through digital twins that synthesize real-time data streams - from traffic patterns to emissions - enabling cities like Sydney to optimize resource allocation and policy design [15–17]. Quantum computing heralds revolutionary potential for sustainability applications, offering exponential computational advantages for carbon capture material design, disaster prediction, and supply chain optimization [18–20]. Concurrently, computational biology supports biodiversity conservation through genomic analysis of endangered species, exemplified by the Earth Biogenome Project's global effort to catalogue eukaryotic life [21,22]. Water resource management achieves unprecedented efficiency through AI-driven systems that reduce agricultural consumption by 27.3 % [23]. Carbon capture technologies leverage computational fluid dynamics to optimize membrane designs, with a 1,700-fold acceleration in simulation workflows [24].

Despite these advancements, critical challenges persist in scaling computational solutions. Hardware constraints, energy demands, and integration barriers hinder quantum computing adoption [20], while ethical considerations – including equitable resource access, data privacy, and community engagement in conservation genomics – demand vigilant attention [5,25]. Realizing the full potential of computational science requires interdisciplinary collaboration among computer scientists, domain experts, policymakers, and communities.

Computational science guides society toward sustainability through interconnected themes, including climate system modeling, renewable energy transitions, digital urbanization, and emerging technologies. In line with this vision, we are delighted to introduce a special issue inspired by the theme "Computational Science: Guiding the Way Towards a Sustainable Society," which stems from the International Conference on Computational Science (ICCS) 2024. This special issue aims to address the current challenges in the pursuit of 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 the arts and humanities. ICCS has been hosted by various institutions and cities across 13 countries, including Australia, Czechia, China, Iceland, Poland, Portugal, Russia, the Netherlands, Singapore, Spain, Switzerland, the United Kingdom, and the United States. Throughout its history, ICCS has always been focused on recent advancements in computational science.

Analyzing the evolution of ICCS topics [26,27] 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. Based on the comprehensive analysis of 24 years of ICCS publications, the topic dynamics reveal profound shifts in the computational science landscape while underscoring enduring foundational pillars (see Fig. 1). Machine learning has emerged as the dominant paradigm, surpassing parallel and distributed computing after 2019 to become the most prevalent topic by 2024, accounting for 20.8 % of ICCS publications. This transformative shift – accelerated by breakthroughs like the

https://doi.org/10.1016/j.jocs.2025.102663

Available online 24 June 2025

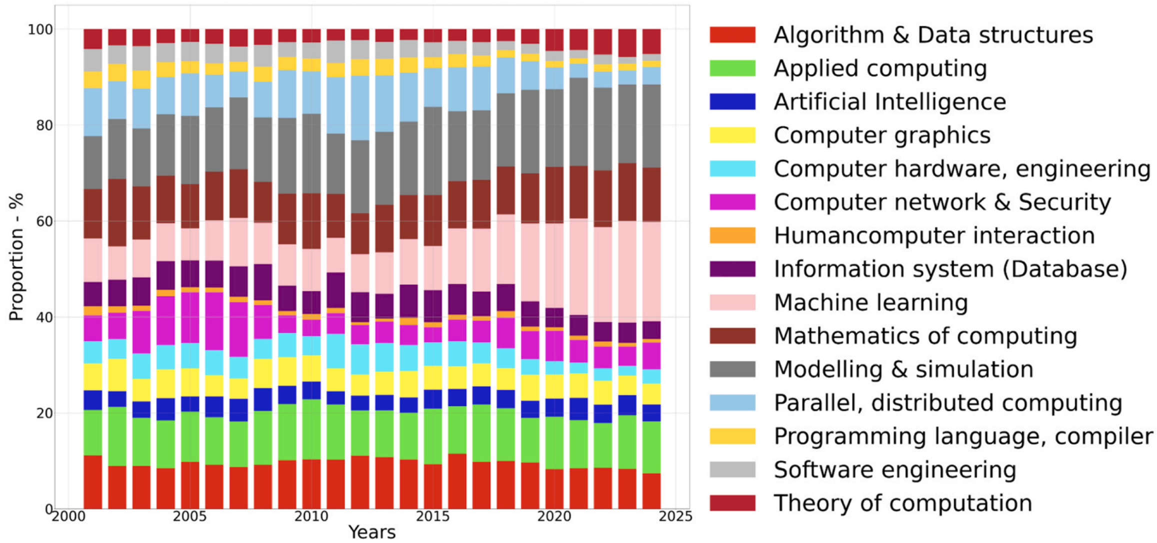

Fig. 1. Percentage of first-level discipline in ICCS over 24 years. Source: Special issue paper [27].

transformer architecture – reflects the community's rapid adoption of AI methodologies. Concurrently, parallel and distributed computing, once the apex topic during the supercomputing race of the early 2010s (peaking at 13.4 % in 2012–2013), has declined to just 3.6 % of research focus by 2024, alongside significant reductions in embedded systems and operating systems. The analysis further identifies four distinct technological disrupts shaping ICCS's evolution: the network era (pre-2007, driven by IPv6 and P2P systems), the parallel computing era (2009–2014, fueled by GPU advancements like CUDA), the big data era (2015–2018), and the current machine learning era (2018–present). Throughout these transitions, three methodological pillars remain central: algorithms, mathematical modeling, and network science consistently rank among the top three topics over 24 years, demonstrating their role as the "irreplaceable foundations" of computational science. Quantum computing has recently surged, entering the top 20 topics in 2024, signaling emerging frontiers. These dynamics highlight the community's dual nature: agile responsiveness to disruptive technologies (e.g., GPUs, transformers) alongside sustained investment in theoretical and algorithmic core competencies. More details on the topic analysis can be found in [27].

The ICCS society continues to attract renowned scientists as well as young researchers. Four years ago, we had the pleasure of announcing a special issue of the Journal of Computational Science [28]. 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. At the same time, ICCS functions as a collaboration incubator: network analysis and modelling reveal that 65.6 % of authors belong to a giant connected component, with 3623 confirmed emergent collaborations originating from conference interactions [27,29]. These partnerships exhibit measurable patterns, with an average 4.8-year latency to first joint publication – demonstrating ICCS's role in seeding sustained research networks. This dual function – curating foundational methodologies while accelerating knowledge diffusion through both structured and serendipitous interactions – solidifies ICCS's position as the central intellectual crossroads for the evolving landscape of computational science.

The evolution of ICCS 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), "Computation at the Cutting Edge of Science" (ICCS 2023). These themes underscore the pivotal role of computational science in addressing contemporary challenges across diverse 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 critical 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.

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 2024 held on July 2–4, 2024 at the University of Málaga, Spain with a special theme "Computational Science: Guiding the Way Towards a Sustainable Society". The 24th edition of the conference, featuring 17 tracks (16 thematic tracks and one main track), and with nearly 300 participants, continues the conference's longstanding commitment to quality and impact. This issue continues the sequence of annual collections of key ICCS publications [30,31]. The presented issue contains extended papers demonstrating the various topics relevant to the ICCS society. These topics were selected from 225 papers published in the ICCS 2024 conference proceedings in Vol. 14832–14838 by Lecture Notes in Computer Science [32], which were chosen from over 440 submissions.

As usual, many ICCS papers report on numerical methods' development, improvement, and implementation, as they form the core of the computational science area. The article by Başsoy [33] presents flexible, high-performance algorithms for Tensor-Matrix Multiplication (TTM) by leveraging BLAS operations, enabling efficient computation across diverse tensor layouts and dimensions. The proposed algorithms achieve near-peak performance, outperforming existing implementations like Intel MKL, Libtorch, and Eigen by significant margins – up to 334 % faster in some cases – while matching or exceeding specialized libraries like TBLIS for real-world tensor workloads. Chinellato and Marcuzzi

[34] proposed a modified Kalman Filter model named Deep Kalman Filter (DKF) that can solve for several regularization strategies data data-driven model estimation quite accurately. Poczekajlo et al. [35] introduce modified CORDIC algorithms that enhance FPGA-based trigonometric computations, improving real-time signal processing and numerical linear algebra applications, with up to 50 % accuracy improvement and a 15 % reduction in latency compared to standard methods.

Another critical aspect of ICCS is the development of advanced solutions in high-performance computing. Piñeiro et al. [36] present MPI4All, a novel tool designed to simplify the development of efficient and comprehensive MPI bindings for any programming language, addressing limitations in existing solutions. The tool ensures full MPI API coverage with minimal effort, automatically updates for future MPI versions, and demonstrates competitive performance in Go and Java compared to state-of-the-art approaches. Williams et al. [37] proposed advanced multi-GPU programming tools to enhance BIT1 plasma simulations related to the operation of nuclear fusion accelerators, such as the ITER tokamak project. Results show significant performance improvements in the range of 53–58 % compared to standard tools. Ryabinin et al. [38] present a novel software architecture for a high-performance direct astrometric solver designed to efficiently handle billions of observations by addressing systematic errors in space telescope data. The results demonstrate that the solver achieves a linear speedup with the number of CPUs and a quadratic scaling with the observation count, successfully processing up to 9.2 billion observations in 8.5 h while maintaining numerical robustness and accuracy. Ichimura et al. [39] propose a method to accelerate and improve the energy efficiency of explicit elastic wavefield simulations on GPUs by leveraging INT8 Tensor Cores and reducing numerical dispersion. The results demonstrate that the proposed GPU-based method outperforms conventional CPU and multi-GPU systems in both speed and efficiency for large-scale simulations.

An important part of computational science is algorithms and software development with a specific attention lately attracted by machine learning and deep learning algorithms. Yan and He [40] proposed a novel Dual Phase Physics-Informed Neural Networks (DP-PINN) that incorporates a set of optimization strategies to enhance its prediction accuracy, particularly in solving complex PDEs such as the Allen-Cahn equation, by significantly reducing prediction errors that accumulate over time. Jajeśniak et al. [41] discuss Interpoint Inception Distance (IID) as a novel method for evaluating deep generative models (DGMs) by measuring discrepancies between multidimensional feature distributions through one-dimensional interpoint comparisons. The key results demonstrate that Cramér Interpoint Inception Distance (CIID) exhibits strong theoretical properties and competitive performance compared to Fréchet Inception Distance (FID), rendering it a promising alternative for DGM evaluation. Świderski and Jastrzebska [42] describe a new dynamically neural network based growing-shrinking algorithm that permits training and adjusting the architecture while the model is being trained. The mechanism for the architectural design is governed by a Monte Carlo tree search procedure, which simulates network behavior and allows comparing several candidate architecture changes to choose the best one. Joy et al. [43] analyze several parameter tuning algorithms applied to the Firefly Algorithm (FA), evaluating it with six different optimization problems. The results demonstrate that the FA's performance and tuned parameter values are independent of the tuning method used (Monte Carlo, Quasi-Monte Carlo, or Latin Hypercube Sampling), as validated by comprehensive statistical analysis.

Highlighting the sustainable society topic, this ICCS event covers a wide range of related application areas. One of the main related areas is computational biomedicine and healthcare. Geddes et al. [44] introduce a method to quantify the effects of modulating temporal arterial waveforms on hemodynamic metrics by extending a "points of interest" approach from coronary arteries to carotid and pulmonary artery waveforms. The results identify critical regions of inlet velocity waveforms that most significantly influence hemodynamics, particularly the secondary peak, and provide a framework for assessing the impact of waveform variations on clinical metrics, such as wall shear stress and oscillatory shear index. Tanade and Randles [45] introduce HarVI, a real-time coronary intervention planning tool that combines machine learning (ML) for hemodynamic prediction and extended reality (XR) for interactive 3D visualization. The results demonstrate that HarVI accurately replicates 1D CFD simulations with a significantly faster turnaround time (62 min on average), enabling same-day intervention planning and a tenfold improvement over existing standards. Liu et al. [46] explore the use of Krylov iterative solvers (CG, MINRES, GMRES) in interior point methods (IPMs) for optimization problems in radiation therapy, addressing challenges like ill-conditioning through preconditioning strategies. The study demonstrates that a doubly augmented KKT system with Jacobi-preconditioned CG and constraint preconditioning for symmetric indefinite systems improves solver convergence, showing promise for GPU acceleration and achieving acceptable accuracy for real-world radiation therapy and support vector machine problems. This study by Shaheen and Melnik [47] combines machine learning, stochastic modeling, and Bayesian inference to analyze brain network dynamics in Parkinson's disease (PD), aiming to improve understanding and treatment strategies. The results show that stochastic disturbances increase thalamus activity in the cortex-basal ganglia-thalamus network, even under deep brain stimulation, and Bayesian inference suggests reducing these disturbances could enhance healthy brain states, offering potential pathways for personalized therapies.

With a focus on environmental modeling, such topics like wildfire spread analysis and prediction form an important application area to computational science. González et al. [48] introduce a new parametric approach using Composite Bézier Curves (CBC) to improve fire perimeter representation in Wildland Urban Interface (WUI) areas, addressing limitations of traditional polygonal models. The results demonstrate that CBC-based methods, particularly CBCD, produce smoother, more realistic fire fronts and enhance fire spread prediction accuracy in complex terrains compared to existing simulators like FARSITE. Carrillo et al. [49] propose using edge computing with low-power GPUs to enable real-time, high-resolution wildfire spread predictions directly in remote areas, reducing reliance on high-performance computing (HPC) platforms. The results demonstrate that this approach can accurately simulate fire spread up to 5 h ahead within minutes, processing data on-site even without internet connectivity, thus improving wildfire management for firefighters.

Transportation, logistics, and other applications of flying vehicles are actively developed for society's needs lately. The study by Magata et al. [50] investigates the aerodynamic effects of wind disturbances on small Urban Air Mobility (UAM) vehicles during high-speed flight, emphasizing the need for accurate flight dynamics models that incorporate drag and torque. The findings reveal that the flight dynamics model underestimates air resistance and must account for drag-induced torque. In contrast, computational fluid dynamics (CFD) simulations show that drag and torque reproduction influence nose-down attitude and local pressure changes during forward flight, with constant-velocity turns being less affected by crosswinds than accelerating turns. Mori et al. [51] investigate Vortex Ring State (VRS) in quadcopter descent, analyzing its occurrence and effects through experiments and simulations. The main results show that large attitude angle changes and lift fluctuations exceeding 15 % occur near the hovering induced velocity, with vortex ring formation and flow stagnation around the rotors leading to instability.

Besides the mentioned major application areas, there are numerous application scenarios where computational science plays a crucial role. Zhang et al. [52] propose a Markov Game-based Defense Timing Selection (MGDTS) approach to enhance Moving Target Defense (MTD) in Satellite Computing Systems (SCSs), optimizing defense timing while considering limited resources and periodic user traffic. Experiments demonstrate that MGDTS reduces resource costs, minimizes disruption to user traffic, and improves security compared to existing MTD strategies. Bekasiewicz et al. [53] propose an automated approach to antenna design that reduces reliance on engineering bias by using variable-fidelity optimization strategies to generate and tune antenna topologies. The main results demonstrate that the framework effectively generates and optimizes antenna designs with minimal high-fidelity simulations, outperforming traditional methods and producing competitive topologies compared to state-of-the-art solutions. Bragone et al. [54] explore the use of machine learning techniques, including PCA and LSTM networks, to analyze and predict the Brownian dynamics of Cellulose Nanofibrils (CNFs) for sustainable material development. PCA and LSTM models effectively predict CNF behavior after flow cessation, while unsupervised learning classifies CNF materials by concentration, and autocorrelation analysis reveals seasonal patterns in lower concentrations. Grycuk et al. [55] introduced a new approach for real-time retrieval and classification of solar images using an image hashing technique. The method, by reducing the amount of data required to describe Sun images, achieves real-time retrieval speed, with several potential applications, such as searching, classifying, and retrieving solar flares, which are of critical importance.

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.

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 (1) (2010) 3–4, https://doi.org/10.1016/j.jocs.2010.04.003.
[2] T. Hey, S. Tansley, K. Tolle, The fourth paradigm: data-intensive scientific discovery, Microsoft Res. (2009).
[3] M.D. Assunção, R.N. Calheiros, S. Bianchi, M.A.S. Netto, R. Buyya, Big data computing and clouds: trends and future directions, vol. 79–80, J. Parallel Distrib. Comput. (2015) 3–15, https://doi.org/10.1016/j.jpdc.2014.08.003.
[4] M. Chen, L. Chen, Y. Li, Y. Xian, Developing computable sustainable urbanization science: interdisciplinary perspective, Comput. Urban Sci. 2 (1) (2022) 17, https://doi.org/10.1007/s43762-022-00048-9.
[5] Y. Kan, AI for environmental sustainability: advances, challenges, and future directions, Int. J. Artif. Intell. Sci. 1 (1) (2025), https://doi.org/10.63619/ijais.v1i1.006.
[6] L.A. Barba, Praxis of reproducible computational science, Comput. Sci. Eng. 21 (1) (2019) 73–78, https://doi.org/10.1109/MCSE.2018.2881905.
[7] S. Koziel, D.E. Ciaurri, L. Leifsson, Surrogate-Based Methods, in Studies in Computational Intelligence, vol. 356, in: S. Koziel, X.-S. Yang (Eds.), Computational Optimization, Methods and Algorithms, 356, Springer Berlin Heidelberg, Berlin, Heidelberg, 2011, pp. 33–59, https://doi.org/10.1007/978-3-642-20859-1_3. in Studies in Computational Intelligence, vol. 356.
[8] D. Lim, Yaochu Jin, Yew-Soon Ong, B. Sendhoff, Generalizing surrogate-assisted evolutionary computation, IEEE Trans. Evol. Comput. 14 (3) (2010) 329–355, https://doi.org/10.1109/TEVC.2009.2027359.
[9] A.A. Funkner, A.N. Yakovlev, S.V. Kovalchuk, 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.
[10] 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 (187) (2022) 20210864, https://doi.org/10.1098/rsif.2021.0864.
[11] T. Nguyen, J. Jewik, H. Bansal, P. Sharma, A. Grover, ClimateLearn: Benchmarking machine learning for weather and climate modeling. Proceedings of the 37th International Conference on Neural Information Processing Systems, in NIPS '23. Red Hook, Associates Inc, NY, USA: Curran, 2023.
[12] S. Partee, et al., Using machine learning at scale in numerical simulations with SmartSim: an application to ocean climate modeling, J. Comput. Sci. 62 (2022) 101707, https://doi.org/10.1016/j.jocs.2022.101707.
[13] B. Kc, Department of Electrical and Computer Engineering, Southern Illinois University of Carbondale, USA, H. Alkhwaildi, and Department of Electrical and Computer Engineering, Southern Illinois University of Carbondale, USA, "Multi-Objective TLBO and GWO-based Optimization for Placement of Renewable Energy Resources in Distribution System,", Comput. Res. Prog. Appl. Sci. Eng. 7 (2) (2021) 1–13, https://doi.org/10.52547/crpase.7.2.2356.
[14] Akram M. Musa, M. Abu-Shaikha, R.Y. Al-Abed, Enhancing predictive accuracy of renewable energy systems and sustainable architectural design using PSO algorithm, Int. J. Comput. Exp. Sci. Eng. 11 (1) (2025), https://doi.org/10.22399/ijcesen.842.
[15] A. Sohail, et al., Beyond data, towards sustainability: a sydney case study on urban digital twins, PFG J. Photogramm. Remote Sens. Geoinf. Sci. (2025), https://doi.org/10.1007/s41064-025-00337-y.
[16] C.R. Corrado, S.M. DeLong, E.G. Holt, E.Y. Hua, A. Tolk, Combining green metrics and digital twins for sustainability planning and governance of smart buildings and cities, Sustainability 14 (20) (2022) 12988, https://doi.org/10.3390/su142012988.
[17] S.M. Homayouni, J. Pinho De Sousa, C. Moreira Marques, Unlocking the potential of digital twins to achieve sustainability in seaports: the state of practice and future outlook, WMU J. Marit. Aff. 24 (1) (2025) 59–98, https://doi.org/10.1007/s13437-024-00349-2.
[18] M. Filipova, G. Gospodinov, L. Gotsev, E. Kovatcheva, B. Jekov, Quantum computing applications for addressing global warming and pollution: a comprehensive analysis, Environ. Technol. Resour. Proc. Int. Sci. Pract. Conf. 1 (2024) 154–160, https://doi.org/10.17770/etr2024vol1.8001.
[19] K.T.M. Ho, K.-C. Chen, L. Lee, F. Burt, S. Yu, P.-H. Lee, Quantum Computing for Climate Resilience and Sustainability Challenges. 2024 IEEE International Conference on Quantum Computing and Engineering (QCE), Montreal, QC, IEEE, Canada, 2024, pp. 262–267, https://doi.org/10.1109/QCE60285.2024.10289.
[20] Management Information Systems, College of business, Lamar University, USA. et al., AI and quantum computing for cafbon-neutral supply chains: a systematic review of innovations, Am. J. Interdiscip. Stud. 6 (1) (2025) 40–75, https://doi.org/10.63125/nrdx7d32.
[21] M.P. Tan, et al., Applications of next-generation sequencing technologies and computational tools in molecular evolution and aquatic animals conservation studies: a short review, p. 1176934319892284, Evol. Bioinforma. 15 (2019), https://doi.org/10.1177/1176934319892284.
[22] J.E.A. Huddart, A.J. Crawford, A.L. Luna-Tapia, S. Restrepo, F. Di Palma, EBP-colombia and the bioeconomy: genomics in the service of biodiversity conservation and sustainable development, Proc. Natl. Acad. Sci. 119 (4) (2022) e2115641119, https://doi.org/10.1073/pnas.2115641119.
[23] Z. Jiang, The impact of sustainable management systems on the sustainable development of water resources in agriculture and the reduction of agricultural carbon footprint, in: S.S. Agaian (Ed.), in Second International Conference on Big Data, Computational Intelligence, and Applications (BDCIA 2024), SPIE, Huanggang, China, 2025, p. 157, https://doi.org/10.1117/12.3059876.
[24] B. Lei, et al., Accelerating computational fluid dynamics simulation of post-combustion carbon capture modeling with MeshGraphNets, Front. Artif. Intell. 7 (2025) 1441985, https://doi.org/10.3389/frai.2024.1441985.
[25] S.A. Miner, T.J. Thurman, Genomics and biodiversity: applications and ethical considerations for climate-just conservation, Hastings Cent. Rep. 54 (S2) (2024), https://doi.org/10.1002/hast.4936.
[26] T.M. Abuhay, S.V. Kovalchuk, K.O. Bochenina, G. Kampis, V.V. Krzhizhanovskaya, M.H. Lees, Analysis of computational science papers from ICCS 2001-2016 using topic modeling and graph theory, Procedia Comput. Sci. 108 (2017) 7–17, https://doi.org/10.1016/j.procs.2017.05.183.
[27] L. Luo, et al., Evolution of the computational science community: the dynamics of topics and collaborations in 24 years of ICCS and JoCS publications, J. Comput. Sci. 89 (2025) 102609, https://doi.org/10.1016/j.jocs.2025.102609.
[28] S.V. Kovalchuk, V.V. Krzhizhanovskaya, P.M.A. Sloot, 20 years of computational science, J. Comput. Sci. 46 (2020) 101187, https://doi.org/10.1016/j.jocs.2020.101187.
[29] N. Dorzhu, T. Sukhomlinova, L. Luo, S. Kovalchuk, Predicting future collaborations in a scientific community using graph neural networks. 25th International Conference on Computational Science, 2025 (p. (in press)).
[30] S.V. Kovalchuk, et al., The computational planet, J. Comput. Sci. 72 (2023) 102102, https://doi.org/10.1016/j.jocs.2023.102102.
[31] S.V. Kovalchuk, et al., Computation at the cutting edge of science, J. Comput. Sci. 81 (2024) 102379, https://doi.org/10.1016/j.jocs.2024.102379.
[32] L. Franco, C. de Mulatier, M. Paszynski, V.V. Krzhizhanovskaya, J.J. Dongarra, and P.M.A. Sloot, "Computational Science – ICCS 2024. Preface," Lect. Notes Comput. Sci., vol. 14832, pp. v–vi, doi: 10.1007/978-3-031-63749-0.
[33] C.S. Başsoy, Design of a high-performance tensor–matrix multiplication with BLAS, J. Comput. Sci. 87 (2025) 102568, https://doi.org/10.1016/j.jocs.2025.102568.
[34] E. Chinellato, F. Marcuzzi, State, parameters and hidden dynamics estimation with the Deep Kalman Filter: regularization strategies, J. Comput. Sci. 87 (2025) 102569, https://doi.org/10.1016/j.jocs.2025.102569.

[35] P. Poczekajlo, L. Moroz, E. Deelman, P. Gepner, Evaluation of new CORDIC algorithms implemented on FPGA for the Givens Rotator, J. Comput. Sci. 87 (2025) 102567, https://doi.org/10.1016/j.jocs.2025.102567.
[36] C. Piñeiro, Á. Vázquez, J.C. Pichel, Towards universal MPI bindings for enhanced new language support, J. Comput. Sci. 87 (2025) 102557, https://doi.org/10.1016/j.jocs.2025.102557.
[37] J.J. Williams, et al., Accelerating particle-in-cell Monte Carlo simulations with MPI, OpenMP/OpenACC and asynchronous multi-GPU programming, J. Comput. Sci. 88 (2025) 102590, https://doi.org/10.1016/j.jocs.2025.102590.
[38] K. Ryabinin, G. Sarras, W. Löffler, O. Erokhina, M. Biermann, AJAS: a high performance direct solver for advancing high precision astrometry, J. Comput. Sci. 87 (2025) 102554, https://doi.org/10.1016/j.jocs.2025.102554.
[39] T. Ichimura, K. Fujita, M. Hori, M. Lalith, Fast and power efficient GPU-based explicit elastic wave propagation analysis by low-ordered orthogonal voxel finite element with INT8 tensor cores, J. Comput. Sci. p. (2025).
[40] D. Yan, L. He, DP-PINN+: a dual-phase PINN learning with automated phase division, J. Comput. Sci. (2025) 102637, https://doi.org/10.1016/j.jocs.2025.102637.
[41] D. Jajeśniak, P. Kościelniak, A. Zajdel, M. Mazur, Deep dive into generative models through feature interpoint distances, J. Comput. Sci. 86 (2025) 102539, https://doi.org/10.1016/j.jocs.2025.102539.
[42] S. Świderski, A. Jastrzebska, Data classification with dynamically growing and shrinking neural networks, J. Comput. Sci. p. (2025).
[43] G. Joy, C. Huyck, X.-S. Yang, Parameter tuning of the firefly algorithm by three tuning methods: standard Monte Carlo, quasi-Monte Carlo and latin hypercube sampling methods, J. Comput. Sci. 87 (2025) 102588, https://doi.org/10.1016/j.jocs.2025.102588.
[44] J.R. Geddes, T.D. King, C. Tanade, W. Ladd, N.S. Khan, A. Randles, Impact of inlet velocity waveform shape on hemodynamics, J. Comput. Sci. 87 (2025) 102579, https://doi.org/10.1016/j.jocs.2025.102579.
[45] C. Tanade, A. Randles, Real-time virtual intervention for simple and serial coronary artery disease using the HarVI framework, J. Comput. Sci. 87 (2025) 102570, https://doi.org/10.1016/j.jocs.2025.102570.
[46] F. Liu, M.I. Andersson, A. Fredriksson, S. Markidis, Preconditioned CG and GMRES for interior point methods with applications in radiation therapy, J. Comput. Sci. p. (2025).
[47] H. Shaheen, R. Melnik, Bayesian approaches for revealing complex neural network dynamics in Parkinson's disease, J. Comput. Sci. 85 (2025) 102525, https://doi.org/10.1016/j.jocs.2025.102525.
[48] I. González, C. Carrillo, A. Cortés, T. Margalef, Realistic wildfire growth simulations applying a differentiable parametric representation of the fire front based on Composite Bézier curves, J. Comput. Sci. (2025) 102640, https://doi.org/10.1016/j.jocs.2025.102640.
[49] C. Carrillo, T. Margalef, A. Espinosa, A. Cortés, Edge computing driven forest fire spread simulation: an energy-aware study, J. Comput. Sci. 88 (2025) 102605, https://doi.org/10.1016/j.jocs.2025.102605.
[50] T. Magata, et al., Forward and turning flight simulation of flying cars and comparative evaluation of flight dynamics models considering wind disturbances, J. Comput. Sci. 85 (2025) 102519, https://doi.org/10.1016/j.jocs.2024.102519.
[51] R. Mori, et al., Flow field analysis of Vortex Ring State through descent experiments and simulations with a quadcopter, J. Comput. Sci. 85 (2025) 102528, https://doi.org/10.1016/j.jocs.2025.102528.
[52] L. Zhang, Y. Guo, S. Leng, X. Cao, F. Li, L. Fang, Defense timing selection for MTD in periodic satellite computing systems: a Markov game approach, J. Comput. Sci. 87 (2025) 102583, https://doi.org/10.1016/j.jocs.2025.102583.
[53] A. Bekasiewicz, K. Askaripour, M. Dzwonkowski, T. Dhaene, I. Couckuyt, Strategies for feature-assisted development of topology agnostic planar antennas using variable-fidelity models, J. Comput. Sci. 85 (2025) 102521, https://doi.org/10.1016/j.jocs.2024.102521.
[54] F. Bragone, K. Morozovska, T. Rosén, T. Laneryd, D. Söderberg, S. Markidis, Automatic learning analysis of flow-induced birefringence in cellulose nanofibrils, J. Comput. Sci. 85 (2025) 102536, https://doi.org/10.1016/j.jocs.2025.102536.
[55] R. Grycuk, R. Scherer, G. De Magistris, C. Napoli, Real-time detection and classification of active regions from solar images using sector-based hashing, J. Comput. Sci. 89 (2025) 102604, https://doi.org/10.1016/j.jocs.2025.102604.

Sergey V. Kovalchuk*
International Conference on Computational Science, the Netherlands

Clélia de Mulatier, Valeria V. Krzhizhanovskaya
University of Amsterdam, Amsterdam, the Netherlands

Leonardo Franco
University of Malaga, Malaga, Spain

Maciej Paszyński
AGH University of Krakow, Krakow, Poland

Jack Dongarra
University of Tennessee, Knoxville, USA

Peter M.A. Sloot
University of Amsterdam, Amsterdam, the Netherlands

* Corresponding author.
E-mail address: sergey.v.kovalchuk@gmail.com (S.V. Kovalchuk).