The computational planet

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1. Introduction

The field of computational science [1] emerged at the crossroads of computer science, information technologies, and mathematical modeling. As a vast interdisciplinary domain, it encompasses a diverse set of methodologies and specific tools to address research challenges across various application areas, spanning from traditional natural sciences to emerging fields like medicine, social sciences, and humanities. Furthermore, computational science paves the way for novel directions and innovative modes of 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].

Moreover, 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].

Thirdly, 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 "The Computational Planet," which stems from the International Conference on Computational Science (ICCS) 2022. 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. As an A-rank conference in the CORE classification, ICCS has been hosted by different institutions and cities across 12 countries, including Australia, China, Iceland, Poland, Portugal, Russia, the Netherlands, Singapore, Spain, Switzerland, the UK, and the USA. Throughout its history, ICCS has focused on recent advancements in computational science.

Analyzing the evolution of ICCS topics [12] 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. Moreover, ICCS remains responsive to emerging technologies and

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approaches, such as the development of GPGPU or IPv6 technologies, as evidenced by the increasing number of publications in these respective areas.

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 [13].

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), and, of course, "The Computational Planet" (ICCS 2022). 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.

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 2022. This issue continues the sequence of annual collections of key ICCS publications [14,15]. The issue contains extended papers demonstrating the various topics relevant to the ICCS society. These topics were selected from 253 papers published in the ICCS 2021 conference proceedings in Vol. 13350–13353 by Lecture Notes in Computer Science [16], which were selected from over 514 submissions.

As usual, many ICCS papers report on **numerical methods** development, improvement, and implementation, as they form the core of the computational science area. Lytaev [17] proposes a new approach to increasing the performance of numerical methods for solving the one-way Helmholtz equation in large-scale domains. Szczęsna et al. [18] present a new procedure to study the dynamics of biomedical signals, which relies on features of a wavelet scattering transform to classify signal segments as either chaotic or non-chaotic. Jaworska [19] presents a new higher order extension of the multipoint meshless finite difference method, which is frequently applied as part of a multiscale model to solve engineering problems.

An important aspect of computational science is represented by papers working with **advanced computational architectures**. Fujita et al. [20] propose an improved tensor-based method for cross-correlation function computation to achieve advanced performance in TensorFloat-32 Tensor Core operations, which are available in the Ampere, Ada, and Hopper architectures. Paul et al. [21] introduced a new programming system for irregular PGAS (Partitioned Global Address Space) applications, in which point-to-point remote operations can be expressed as fine-grained asynchronous actor messages.

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 AI). Also, this part includes original algorithms introduced within the computational science area. Heisler et al. [22] propose an original domain specific language and code generation framework (Finch) for partial differential equations with investigation in finite volume and finite element methods. Li and Deng [23] present an application of the recently developed Soft Iso-Geometric Analysis method (sofIGA) to the three-body problem in quantum mechanics, and study its performance in comparison to the classical IGA method. Campos et al. [24] present a surrogate modeling approach to accelerate uncertainty quantification and global sensitivity analysis for the Holzapfel-Ogden model of cardiac tissue. Phab et al. [25] investigate the ability of quantum computers to attack a toy block cipher using the Quantum Approximate Optimization Algorithm on gate-based quantum computers and a variant of the Quantum Annealing algorithm on analog quantum computers.

A significant sub-area of algorithms is covered by evolutionary computations. Żychowskia and Mańdziuk [26] propose a novel coevolutionary method for solving Stackelberg Security Games (SSGs) with high time efficiency and scalability with near-constant computation time irrespective of the game size. Seredyński et al. [27] presents a theoretical framework called a Competitive Coevolutionary Cellular Automata-based System, which can be used to automatically optimize large distributed systems.

Another important sub-area include machine learning algorithms and solutions within computational science. Bielak et al. [28] investigate a new problem of learning attributed graph embeddings as an extension of structural node embedding and propose an original method for compound node embedding management for various problems such as link prediction. Burkhart and Ruiz [29] tackle the problem of heterogeneous treatment effects in the context of causal inference, by combining a genetic algorithm with a neural network for learning feature representations. Furmańczyk et al. [30] compare several classification methods for positive-unlabelled data based on posterior probability estimation, and assesses their stability and efficiency.

While the two 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. Mycka et al. [31] investigate a problem of music generation with the use of evolutionary algorithms and original design of modular fitness function to achieve technically and aesthetically quality of generated music. Shubyn et al. [32] propose an approach for autonomous guided vehicles management with distributed knowledge federated learning showing improvement in the performance of signal prediction. Cholodowicz and Orlowski [33] explore the use of neuronal network controllers with weight switching to obtain the robust control of inventory systems with perishable goods and uncertain demand. Tanade et al. [34] develop a massive parallel cellular automaton model of 3-dimensional tumor growth to study the influence of cell heterogeneity.

A specific application area recently gain attention is related to the **pandemic of COVID-19**, which is affecting many aspects of our lives since the beginning of 2020. Computational scientists also investigate various aspects of pandemics development and changes introduced by it. Wise et al. [35] presents a case study of the impact of the simulated population size, using a model of the spread of COVID-19 among districts in Zimbabwe and find that different geographical dynamics of the spread of disease are associated with varying population sizes. Guggilam et al. [36] investigate a problem of anomaly detection in high-dimensional time series data with application to the analysis of COVID-19 data and further interpretation of identified anomalies.

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.

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