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20 years of computational science: Selected papers from 2020 International Conference on Computational Science

1. Introduction

Computational science [1] is currently developing as a large multidisciplinary scientific direction where multiple areas are joined together. Initially appeared at the intersection of computer science, information technologies, and mathematical modeling, it is providing new methods and tools for researchers in many fields, from traditional natural sciences to new applications in medicine, social sciences, and humanities. Moreover, computational science is aimed not only toward building solutions to existing domain problems. It provides new approaches and opens new directions in the research, industry, regulation, etc. (see, e.g., Simulation-Based Engineering Science [2]).

Computational science combines two principal scientific approaches organized around a computational experiment. First, the computational experiment is designed and developed in accordance with the domain knowledge and problem definition, forming a deductive or knowledge-based inference of models and computational solutions. Second, the data-driven approaches and methods can be considered as inductive (empirical) inference. The combination of these approaches with wide availability of computational resources gives computational science a boost to develop new and adapt existing general-purpose concepts and technologies. Initially, the research field was based on the intersection of mathematical modeling algorithms (including numerical simulation) and computational-intensive solutions (including high-performance, distributed, hybrid, etc. computing). The development of technologies provides new ways to resolve the existing issues in the area. For example, there is a large amount of data collected through observation, measurement, or as a result of earlier modeling and simulation. These data provide a significant source for scientific discovery, and some authors consider this as a new paradigm (data-intensive scientific discovery) [3]. Together with BigData concepts as a technological backbone, these approaches took their place in the computational science area [4]. Artificial intelligence and machine learning methods recently attracted significant attention within the scientific society and can be considered as another example of such an extension. Within the domain of computational science, these methods may be used for a) management of complex models; b) substitute of computationally-intensive models; c) exploration or interpolation of model parameters and data; d) prediction of model characteristics (including performance, uncertainty, etc.). An example of a powerful such method is surrogate modeling [5,6].

One of the important application areas of computational science is multidisciplinary studies, where a combination of models may provide a comprehensive view of the nature of systems and phenomena. For example, the concept of system-level science [7] considers a holistic description of a system to provide the ability for analysis and computational experiments with different goals using the same solution. Moreover, with the help of computational science, many classes of systems could be described through modeling and simulation, including complex systems [8,9] and global systems [10].

The International Conference on Computational Science (ICCS)[1] brings together researchers and scientists working in fundamental computer science disciplines and in various application areas, who are pioneering computational methods in sciences such as physics, chemistry, life sciences, and engineering, as well as in arts and humanities. Since its inception in 2001, ICCS forms a space where the problem domains, IT, and modeling join together to discuss the present and future research directions. With the 20th ICCS, we were celebrating the 20 years of highly successful conferences and an active society built around the conference. During the past years, the conference was hosted by a variety of institutions and cities in 12 countries across the globe: Australia, China, Iceland, Poland, Portugal, Russia, the Netherlands, Singapore, Spain, Switzerland, UK, USA. The conference was always focused on the recent advances in computational science. Analysis of ICCS topics evolved through its history [11] shows that a significant amount of the works presented in the conference are concentrated around key sub-areas of computational science, including modeling and simulation, high-performance and distributed computing, and numerical methods. Moreover, ICCS reacts to emergent technologies and approaches like the development of GPGPU or IPv6 technologies, which was followed by the growing presence of works in these respective areas.

The ICCS society always attracts both well-known scientists and young researchers. During the previous years, more than 120 (!) leading scientists in the area gave invited talks, tutorials, and lectures as a valuable contribution to the conference. Twelve of them contributed to the conference more than once, bringing the evolution of their ideas to empower ICCS content. It was our pleasure to announce a special issue of the Journal of Computational Science with 12 selected papers prepared by the leading scientists in the area (acting as keynote speakers during ICCS history) and their colleagues, reflecting the vision of issues, recent advances, challenges, and solutions in various sub-areas [12].

[1] http://www.iccs-meeting.org.

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2. Insights from conference ranking

ICCS is an A-rank[2] conference in the CORE classification. During the regular status update, the conference organizers performed an analysis of the scientific community built around the ICCS. Within this section, we would like to share some insights and facts revealed during the last analysis round where ICCS was compared to other conferences and journals in the field.

Computational science as an interdisciplinary field integrates knowledge in (1) computer science, including algorithms, numerical methods, evolutionary and swarm computing, methods and environments for parallel computations; (2) modeling and simulation, including mathematical modeling, computational mechanics, biomechanics, computational geosciences, material science; (3) engineering, including computer-aided design, optimization of scientific codes, design, and development of computer systems. Along these lines, we query a list of journals covering these sub-fields, using the keywords: (Computing OR Computational OR Computation OR (Computer AND Systems) OR (Computer AND Applications) OR (Computer AND Applied)). After careful selection of top journals results, we obtained the following list (in alphabetic order):

Computational Geosciences	IEEE Transactions on Evolutionary Computations
Computational Material Science	IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems
Computational Mechanics	Journal of Computational Science
Computer Methods in Applied Mechanics and Engineering	Journal of Parallel and Distributed Computing
Computers and Mathematics with Applications	Parallel Computing, Swarm and Evolutionary Computation
Future Generation Computer Systems	

We look at the Editors-in-Chief or Founding Editors of these journals and how often they published at the International Conference on Computational Science compared to other venues and journals. We employed the portal.core.edu.au/core-tools/wpp tool from the CORE ranking website, using the query (in alphabetic order):

Luca Benini	Jean-Luc Guermond	Peter M. A. Sloot
Jinjun Chen	Alfons G. Hoekstra	Per Stenström
Carlos A. Coello Coello	Thomas J.R. Hughes	Ponnuthurai N. Suganthan
Swagatam Das	J. Tinsley Oden	David W. Walker
Clint Dawson	Viktor K. Prasanna	Mary F. Wheeler
Leszek F. Demkowicz	Sanjay Ranka	Peter Wriggers
Jack J. Dongarra	Chi-Wang Shu	Xin-She Yang
Rajesh K. Gupta	Susan B. Sinnott	Albert Y. Zomaya

The "where people publish" (WPP) tool by CORE[3] shows that ICCS is the top publication place for these experts in the field of computational science (see Fig. 1). Also, we were proud to see that ICCS is more popular than other CORE conferences and Web of Science indexed journals. It is just after the arXiv repository CORR[4] in the ranking (see Fig. 2).

3. Overview of the virtual special issue

We are glad to present this virtual special issue (VSI) of the Journal of Computational Science with selected extended papers from ICCS 2020. This VSI continues the sequence of annual collections of key ICCS publications [13,14]. The issue contains extended papers demonstrating the various topics relevant to the ICCS society. These manuscripts were selected from more than 350 papers published in the ICCS 2020 conference proceedings in Vol. 12137–12143 by Lecture Notes in Computer Science [15], which were selected from over 700 submissions to the Main Track of the conference and a series of thematic tracks. As usual, the current collection of selected papers belongs to multiple areas within computational science.

As usual, a large portion of works in ICCS is represented by numerical methods development, improvement, and implementation. Łoś et al. [16] consider Stokes system of equations and propose isogeometric residual minimization method with discontinuous Galerkin formulation. Lyman and Iaccarino [17] investigate ways to overcome existing challenges in polynomial chaos methods. Singh and Mehra [18] present an efficient numerical method to quantify the uncertainty in the solution of stochastic fractional integro-differential equations. Emmendorfer and Dimuro [19] introduce a novel point interpolation algorithm that is computationally efficient for diverse types of applications.

One of the popular directions in this area is formed by works related to finite element methods (FEM). Bołtuć and Zieniuk [20] solves the problems with inclusions and non-homogeneous domains using Bézier surfaces using parametric integral equations system method (PIES) and Bézier surfaces. Also, Kapturczak and Zieniuk [21] propose the inclusion of NURBS curves into the mathematical formalism of the PIES for boundary shape modeling. Geronzi et al. [22] propose an approach to tackle complex one-way fluid structure interaction with FEM.

Another quite important direction for data-driven solutions is represented by works tackling data assimilation (DA) techniques. Nino-Ruiz [23] proposes and develops an optimization method for non-Gaussian DA using three-dimensional-variational (3D-Var) cost function to estimate posterior modes of error distributions. De Luca et al. [24] introduce the developed GPU-based recursive filtering algorithm for DA.

A significant number of works is devoted to the development of software and algorithms for computational experiments, including high-performance and distributed computing, problem-solving environments, etc. Do et al. [26] discuss the performance evaluation of hybrid scientific workflows with the proposed lightweight metric for assessing resource usage efficiency of an in situ workflow execution. Huber et al. [27] introduced an approach to parallel multi-core computing using a dependency graph-driven view of the algorithm and applied it to efficiently map the execution process to the underlying platform. Sahasrabudhe et al. [28] investigated the ways of performance improvement in Hypre solver for manycore and GPU architectures. Peng et al. [25] discuss issues of scientific software testing and consider unit and regression tests applied to U.S. EPA's Storm Water Management Model.

Data-driven and machine learning approaches have recently become widely applied in different problems solved by computational science. Maslyaev et al. [29] propose an approach for the data-driven derivation of a partial differential equation using evolutionary computations. Cebrian and Moure [30] introduces a new algorithm for column-level segmentation of depth images based on the RDP split-and-merge strategy. Grzyb et al. [31] present and investigate a new ensemble method for imbalanced data stream with concept drift classification.

Being a multidisciplinary domain, computational science finds multiple areas where brand-new applications can be developed using the existing approaches to model and simulate various classes of systems. For example, one of the popular problem domains is medicine and healthcare. Settino et al. [35] present an integrative data analysis for the identification of prognostic markers for multiple myeloma. Derevitskii et al. [34] describe a novel hybrid modeling approach applied to medical complications prediction with an example of thyrotoxic atrial fibrillation. Sun et al. [36] applied an originally developed finite-element method for cardiovascular fluid–structure interaction modeling. The Internet of things (IoT) and physical infrastructure management also are tightly interconnected with computational science. Lago et al. [33] introduced an experimental study on a conversational interface to manage non-trivial IoT systems. Ernst et al. [32] propose a novel approach to reactive power compensation for dynamically dimmed

[2] http://portal.core.edu.au/conf-ranks/952/.
[3] http://portal.core.edu.au/core-tools/wpp/.
[4] https://arxiv.org/corr.

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The individuals that publish at this conference are: Jack J. Dongarra(11),
Peter M. A. Sloot(7), Alfons G. Hoekstra(7), Viktor K. Prasanna(1), Xin-She
Yang 0001(3), Albert Y. Zomaya(2), Ponnuthurai N. Suganthan(2), Sanjay
Ranka(1), Mary F. Wheeler(1), Luca Benini(1)

In 2016, there were 6 publications by 4 individuals: Jack J. Dongarra, Peter
M. A. Sloot, Alfons G. Hoekstra, Viktor K. Prasanna
In 2017, there were 14 publications by 7 individuals: Luca Benini, Jack J.
Dongarra, Peter M. A. Sloot, Sanjay Ranka, Alfons G. Hoekstra, Xin-She Yang
0001, Ponnuthurai N. Suganthan
In 2018, there were 4 publications by 3 individuals: Albert Y. Zomaya, Jack J.
Dongarra, Peter M. A. Sloot
In 2019, there were 4 publications by 4 individuals: Alfons G. Hoekstra, Xin-
She Yang 0001, Mary F. Wheeler, Albert Y. Zomaya
In 2020, there were 6 publications by 4 individuals: Alfons G. Hoekstra, Xin-
She Yang 0001, Jack J. Dongarra, Peter M. A. Sloot

10 out of the 24 individuals published at this conference in 1 or more years
5 out of the 24 individuals published at this conference in 2 or more years
4 out of the 24 individuals published at this conference in 3 or more years
3 out of the 24 individuals published at this conference in 4 or more years
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Fig. 1. CORE WPP tool report.

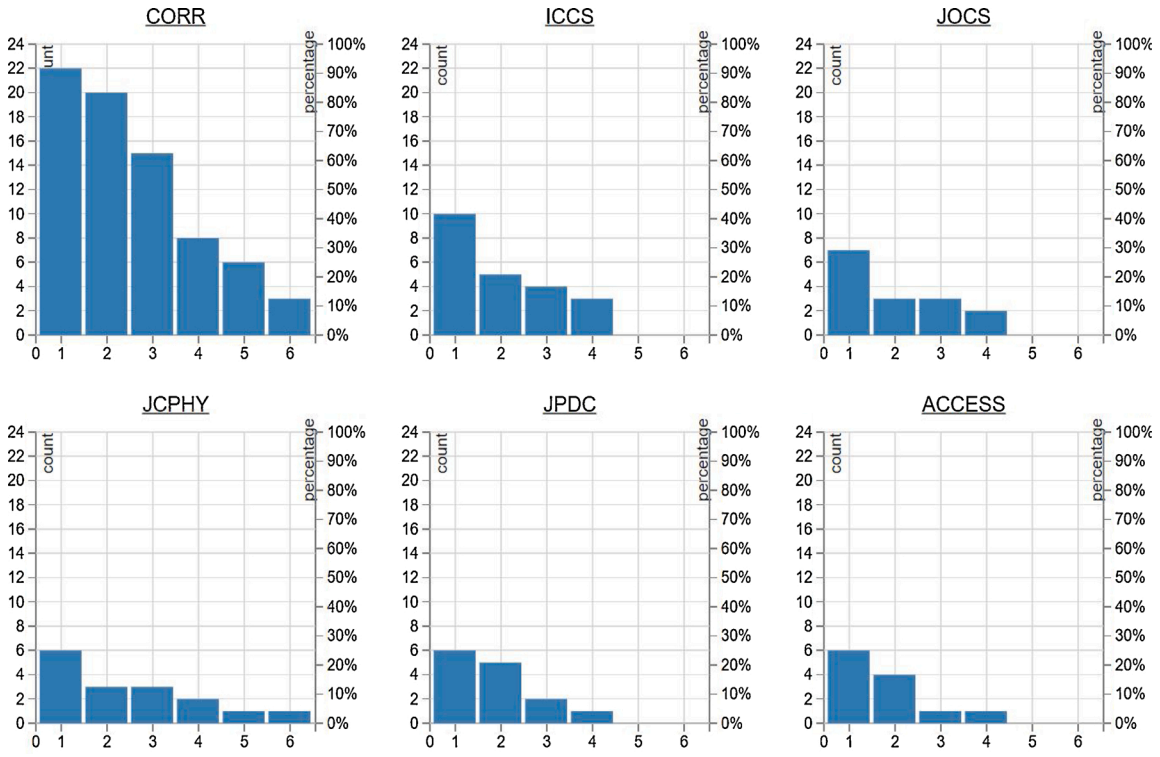

Fig. 2. Top publication places for experts in the field of computational science: ICCS is the first place after the arxiv repository CORR.

LED-based street lighting installations. The list of the areas is large, open, and continues to extend with new ways of computational science application in industry, engineering, etc. Zheng et al. [37] use finite element analysis, Voronoi diagram, and conformal mapping for cost-effective 3D printing of stiffened thin-shell objects. Bocewicz et al. [38] provide a solution to the original milk-run vehicle routing and scheduling problem by considering it as a fuzzy constraint satisfaction problem.

In our opinion, the selection of the papers presented in this VSI represents the state-of-the-art of computational science and its dynamics. We believe that the papers can be of significant interest to the wider scientific community both from the field of computational science and the domains of its application. Also, during the severe pandemic conditions, we consider this VSI as an extended way of communication and discussion in the ICCS community and beyond.

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.

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