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Computational Science in the Interconnected World: Selected papers from 2019 International Conference on Computational Science

1. Introduction

With the roots in computer science and applied mathematics, the computational science (CS) discipline is a fulcrum that brings together general sciences playing a major role in nowadays society. By the exploration of modelling and simulation through advanced computational methodologies, CS touches vast fields of knowledge originating a high demand of practitioners by all organization's types. In this context, practitioners come to intermingle, collaborate, and share resources and visions, building a large multidisciplinary community, thriving to solve highly complex computational problems, which were only dreamed by a few some years ago.

In its line of action, for instance, CS is used to simulate phenomena that would be prohibitive because of many kinds of impracticalities such as cost or danger. The investigation starts by identifying a real problem or phenomenon which is simplified to an abstraction model. The abstract model is then transformed to a computation model by moving it to formal mathematics and algorithms. Algorithms are later implemented in some programming code, used in the final step to run the simulations of the original problem. Simulations allow a controlled scenario, that can be repeated with different parameters, starting points, and conditions in general, most certainly diminishing the associated costs when compared to executing the real scenario. Increasing computational capacities, new algorithms, and methods, allow to achieve high production scenarios, making CS a relatively recent cane for science, completing the theoretical and experimental settings known for other sciences. These achievements are supported using from commodity computers to powerful computers [1,2], built over high performance systems constituted by thousands of dedicated nodes, optimised location relative to network and environmental issues, power consumption, security etc.

Against this background, the International Conference on Computational Science (ICCS), annually held since 2001, has grown to become a major event in the CS field, with hundreds of experts meeting and discussing their works, along with keynote lectures presented by world's renowned researchers. In the 2019's edition, the motto was *Computational Science in the Interconnected World*, highlighting the role of CS in an increasingly unified planet. As matter of fact, the context in which this editorial paper is being written, just a few months after the declaration of the COVID-19 pandemic, highlights the importance of this interconnected world and keeps CS in the forefront of the needs, reflected in the epidemiological research that is supported in computational methods [3–6] or the proved accuracy of many disease propagation models [7–12]. In short, CS practitioners work on the knowledge fringe, making this research field very attractive to new and old practitioners,

obliged to solve modern gratifying and intricate computational problems.

2. Overview of the virtual special issue

ICCS 2019, the 19th Annual International Conference on Computational Science, was held on June 12–14, 2019 in Faro, Portugal. The virtual special issue (VSI), entitled *Computational Science in the Interconnected World: Selected papers from 2019 International Conference on Computational Science* [13], maintains the sequence of key publications collections associated to the recent ICCS events, containing a restricted selection of papers, extended from the ones published in the conference's proceedings [14–18]. ICCS 2019 accounted for 573 submissions divided in 228 submissions to the main track and 345 to the workshops, being accepted a total of 233 papers, 65 (28 % accept rate) full papers from the main track and 168 (49 %) full papers from the workshops. For this VSI, 10 papers were selected from the main track and 6 from workshops. Authors were demanded to extend the original submission with at least 40 % new content, describing mature and complete results, followed by a full review process.

The VSI submissions are not devoted to a single field of research, although some majors can be identified. For instance, in the field of high-performance and distributed computing Ames et al. [19] present a distributed GPU-accelerated fluid structure interaction simulations of high hematocrit cell-resolved flows with over 17 million red blood cells. Scaling is compared on a fat node system with six GPUs per node and on a system with a single GPU per node. Through comparison between the CPU- and GPU-based implementations, data movement in multiscale multi-grid FSI simulations on heterogeneous systems costs are identified, proving to be a major performance bottleneck on the GPU. In [20], Fujita et al. develop a study on the acceleration of the element-by-element kernel in matrix-vector products, essential for high-performance in unstructured implicit finite-element applications. Their study pays attention to random data access with data recurrence as major issue to attain performance, proposing a method to avoid these data races for high performance on many-core CPU architectures with wide single instruction, multiple data (SIMD) units, exemplified by finite-element earthquake simulations.

Research on numerical analysis and methods is presented in [21], where Fan, Qiao, and Sun study a thermodynamically consistent, and robust numerical scheme for the dynamical modelling of composition variation in the framework of the modified Helmholtz free energy coupling with the realistic equations of state. Being computationally efficient and memory saving, the scheme was proved to be

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unconditionally stable, being the implementation based on the single-component system, and does not require to choose a reference species for multicomponent fluids. In the same context, Alekseev et al. [22] proposed an instance of epistemic uncertainty quantification concerning the estimation of the approximation error norm is investigated using the ensemble of numerical solutions obtained via independent numerical algorithms. The ensemble of numerical results obtained by five OpenFOAM solvers is analyzed.

In the field of agent simulation and complex systems, Leonenko et al. [23] study an agent-based model for the influenza propagation. The work commits to assess the applicability of the model over a previous influenza incidence and to demonstrate the influence of human contact patterns on the simulated influenza dynamics. Authors use several types of synthetic populations (e.g., intensive mixing of people occurs vs. less variety of contacts) reaching different intensities of influenza outbreaks, concluding that contact patterns may dramatically alter the course of epidemics. Andelfinger et al. [24] propose a passenger model to measure the effect of different public transport vehicle layouts on the required time for boarding and alighting. The model includes a mechanism to emulate rotation behaviour while avoiding complex geometric computations, allowing to perform collision prediction in low density environments. The boarding and alighting model is validated against real experiments from the literature, demonstrating small deviations to the known values. Simulation times for three autonomous vehicle interior layouts proposed by industrial designers in low- and high-density scenarios.

Application to earth and natural process simulations are proposed by Mills et al. [25] which use computational methods to examine the possible consequences of sea level rise, namely salt intrusion and an increase in water volume affect the hydrodynamics and flooding areas of a major estuary in the Iberian Peninsula. The implementation of the devised 2D model simulated the Guadiana Estuary in different scenarios of sea level rise combined with different freshwater flow rates considering varying tidal amplitudes, finding an increase in salinity in all areas around the estuary in response to an increase in mean sea level. Increase in flooding areas around the estuary was also positively correlated with an increase in mean sea level. Assad et al. [26] evaluated the mesoscale ocean circulation aspects of the Brazilian Equatorial margin using a ten-year hydrodynamic back testing, successfully representing *in situ* and satellite data. Results point to aspects such as the north Brazil current influences on the Amazon River plume's shape and spread, and the relationship between the seasonal behaviour of the Inter-tropical convergence zone migration and of the northern branch of the south Equatorial current with the north Brazil current pattern. Also in the simulation field, in [27], Takii et al. present a six degrees of freedom flight simulation with conversion between airplane and helicopter modes as an application for realizing digital flight of a tiltrotor aircraft. The paper considers components such as rotors, engine nacelles, fixed wings, and a fuselage. To perform large deformations of mesh geometry, the computational domain is decomposed into multiple domains corresponding to each of the component, which are independently moved to perform the characteristic behaviour of a tiltrotor aircraft. The airframe is treated as a rigid body, and the coupled simulations considering interaction with surrounding fluid of the aircraft are demonstrated. The result shows complicated fluid phenomena around the tiltrotor aircraft that occur when it flies with mode change.

On data science and artificial intelligence, Begy et al. work [28] envisages assisting data-intensive distributed job scheduling in computational grids. The study proposes a multiple linear regression remote access throughput forecasting model, applicable to large computing workloads, which was derived from experimentally identified remote data access throughput parameters and the statistically tested formalization of those parameters. One of the work's goals is to optimise the network load over different data access methodologies exhibiting nonoverlapping throughput bottlenecks. Kadupitiya et al. [29] explore the idea of using machine learning surrogates to enhance the usability of

molecular dynamics simulations of soft materials for both research and education. In this context, they integrate the machine learning methods with high-performance computing to enhance their predictive power. To demonstrate their approach a parallelised molecular dynamics simulation of self-assembling ions in nanoconfinement is used. They conclude that the implemented regression model, supported on an artificial neural network, successfully learns nearly all the interesting features associated with the output ionic density profiles over a broad range of ionic system parameters.

In the fields of operational research and soft computing, Randall, Montgomery, and Lewis [30] introduce a temporally augmented version of a water management problem which allows farmers to evaluate sustainable crop choices over long time horizons, over projected changes in precipitation and temperature. They use a multiple objective formulation solved by a differential evolution algorithm. Among other conclusions, the authors suggest that, for the studied region, into the future it will no longer be sustainable to grow crops that are grown now, nor in the same quantities. Lima and Adi [31] introduce two new combinatorial optimization problems involving strings, namely, the chain alignment problem and the multiple chain alignment problem. While for the first problem a polynomial-time algorithm using dynamic programming is presented, the former one is proved to be NP-hard, being proposed three heuristics to approximate instances solutions. The proposed heuristics are assessed with simulated data and the applicability of both problems is proven by their results over a gene identification problem variant. Oulamara et al. [32] study a variant of dial-a-ride problem encountered in a mobility service operated by a private company. Customers ask for a transportation service and get a real-time answer about whether their requests are accepted or rejected, maximizing the number of accepted requests while satisfying constraints. Authors propose some reinsertion techniques to exploit solutions' neighbourhoods, which are based in destruction, repair, and ejection operators. Their proposal was tested on real and hard instances provided by the company. In [33], Dur et al. present a weak constraint Gaussian process model to integrate noisy inputs into the classical Gaussian process predictive distribution. To implement a high-performance computing environment, parallelism is explored by defining a parallel weak constraint Gaussian process model which is based on domain decomposition. Then, the algorithm is used for an optimal sensor placement problem and experimental results are provided for pollutant dispersion within a real urban environment. da Silva et al. [34] profile and analyze the power consumption of two production scientific workflow applications executed on distributed platforms. Their work examines the CPU utilization and I/O operations impact on energy usage, as well as the impact of executing multiple tasks concurrently on multi-socket, multi-core nodes. They find that power consumption is impacted non-linearly by the way in which cores in sockets are allocated to workflow tasks and that I/O operations have significant impact on power consumption, helping them to propose a power consumption model which accounts for I/O intensive workflows.

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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