Transactions on Computational Science and Computational Intelligence

Hamid R. Arabnia · Leonidas Deligiannidis
Michael R. Grimaila · Douglas D. Hodson
Kazuki Joe · Masakazu Sekijima
Fernando G. Tinetti *Editors*

Advances in Parallel & Distributed Processing, and Applications

Proceedings from PDPTA'20, CSC'20, MSV'20, and GCC'20

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Transactions on Computational Science and Computational Intelligence

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Volume I and II

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Preface

It gives us great pleasure to introduce this collection of papers that were presented at the following international conferences: Scientific Computing (CSC 2020); Parallel & Distributed Processing Techniques and Applications (PDPTA 2020); Modeling, Simulation & Visualization Methods (MSV 2020); and Grid, Cloud, & Cluster Computing (GCC 2020). These four conferences were held simultaneously (same location and dates) at Luxor Hotel (MGM Resorts International), Las Vegas, USA, July 27–30, 2020. This international event was held using a hybrid approach, that is, "in-person" and "virtual/online" presentations and discussions.

This book is composed of ten Parts. Parts I through IV (composed of 27 chapters) include articles that address various challenges in the area of scientific computing (CSC). Parts V through VII (composed of 31 chapters) include articles that discuss advances in the area of parallel and distributed processing (PDPTA). Recent progress in the fields of modeling, simulation, and visualization methods (MSV) appear in Parts VIII through IX (composed of 17 chapters). Lastly, Part X (composed of 10 chapters) presents advances in grid, cloud, and cluster computing (GCC).

An important mission of the World Congress in Computer Science, Computer Engineering, and Applied Computing, CSCE (a federated congress to which this event is affiliated with), includes *"Providing a unique platform for a diverse community of constituents composed of scholars, researchers, developers, educators, and practitioners. The Congress makes concerted effort to reach out to participants affiliated with diverse entities (such as: universities, institutions, corporations, government agencies, and research centers/labs) from all over the world. The congress also attempts to connect participants from institutions that have* ***teaching*** *as their main mission with those who are affiliated with institutions that have* ***research*** *as their main mission. The congress uses a quota system to achieve its institution and geography diversity objectives."* By any definition of diversity, this congress is among the most diverse scientific meeting in the USA. We are proud

to report that this federated congress had authors and participants from 54 different nations representing variety of personal and scientific experiences that arise from differences in culture and values.

The program committees (refer to subsequent pages for the list of the members of committees) would like to thank all those who submitted papers for consideration. About 50% of the submissions were from outside the USA. Each submitted paper was peer reviewed by two experts in the field for originality, significance, clarity, impact, and soundness. In cases of contradictory recommendations, a member of the conference program committee was charged to make the final decision; often, this involved seeking help from additional referees. In addition, papers whose authors included a member of the conference program committee were evaluated using the double-blind review process. One exception to the above evaluation process was for papers that were submitted directly to chairs/organizers of pre-approved sessions/workshops; in these cases, the chairs/organizers were responsible for the evaluation of such submissions. The overall paper acceptance rate for regular papers was 20%; 18% of the remaining papers were accepted as short and/or poster papers.

We are grateful to the many colleagues who offered their services in preparing this book. In particular, we would like to thank the members of the Program Committees of individual research tracks as well as the members of the Steering Committees of CSC 2020, PDPTA 2020, MSV 2020, and GCC 2020; their names appear in the subsequent pages. We would also like to extend our appreciation to over 500 referees.

As sponsors-at-large, partners, and/or organizers, each of the followings (separated by semicolons) provided help for at least one research track: Computer Science Research, Education, and Applications (CSREA); US Chapter of World Academy of Science; American Council on Science and Education & Federated Research council; and Colorado Engineering Inc. In addition, a number of university faculty members and their staff, several publishers of computer science and computer engineering books and journals, chapters and/or task forces of computer science associations/organizations from three regions, and developers of high-performance machines and systems provided significant help in organizing the event as well as providing some resources. We are grateful to them all.

We express our gratitude to all authors of the articles published in this book and the speakers who delivered their research results at the congress. We would also like to thank the followings: UCMSS (Universal Conference Management Systems & Support, California, USA) for managing all aspects of the conference; Dr. Tim Field of APC for coordinating and managing the printing of the programs; the staff of Luxor Hotel (MGM Convention) for the professional service they provided; and Ashu M. G. Solo for his help in publicizing the congress. Last but not least, we would like to thank Ms. Mary James (Springer Senior Editor in New York) and

Arun Pandian KJ (Springer Production Editor) for the excellent professional service they provided for this book project.

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Part I
Military and Defense Modeling and Simulation

Julia and Singularity for High Performance Computing

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1 Introduction

Our research team is focusing on developing a software suite of tools to simulate quantum systems, specifically in regard to quantum teleportation. Our goal is to create a library general enough for researchers to be able to apply our software to many different quantum problems rather than one specific one and to keep it as open source and distributable as possible. Due to the high level of computation needed to fully model these systems, code run-times can easily and exponentially be driven upward as the matrices involved become increasingly larger.

High-level dynamic languages such as Python, despite their benefits in ease of use and readability, simply do not offer the speed we require. However, lower-level languages such as C offer considerably less flexibility and greater difficulty in developing and maintaining code. As a middle ground to this, we have chosen to use the relatively newer programming language Julia. Julia, while being a dynamic language, was developed with speed in mind, targeting researchers and data scientists hoping to get as much performance out of their code as possible while still maintaining inherit readability and ease of use. This made it an obvious first choice for our research.

Also, due to the high level of matrix calculations involved in quantum mechanics, our research can benefit greatly from the performance gains offered by running as much of our code as possible on GPUs rather than the traditional CPU. Julia offers an extensive amount of support in this area, as it has native GPU programming capabilities offered by the CUDAnative.jl library, as well as multiple other libraries

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for support. Combined with Julia's just-in-time compiler, these libraries offer a great level of efficiency in the kernel launch sequence.

In keeping distributability in mind, we have also opted to develop our library inside of the container engine Singularity. Collaborators can be limited by local security practices and administrative privileges needed to install dependencies required to run the software and code of others. This is combined with the need to maintain version control of software libraries fundamental to their own workflow. Containerization as a technology has risen to meet these needs. Containers offer similar benefits to virtual machines such as managing library dependencies and running multiple isolated operating systems (OS) from the same machine. They do, however, have certain advantages more critical to our work.

Specifically, Singularity makes use of a definition file, where software such as the operating system and essential libraries are defined. This allows us to share our work with others, ensuring all versions and libraries will exactly match our own without interfering with their workflow. This also offers a kind of version control for our work and makes it easier to develop on one machine and execute on another. All that is required is to simply build the container from the definition file, and everything that is required will be installed without having to worry about system administration. Companies such as NVIDIA also offer large repositories of containers pre-built to meet many different needs, allowing us and other researchers to further focus on our research.

Another key benefit we see in using containers is their ability to directly share the kernel of the host OS without the need for a hypervisor, defined later, as is required for a virtual machine. This allows them to directly access the resources of a physical machine with minimal overhead. This is crucial, as much of our code will revolve around utilization of GPUs and getting as much of their speedup as possible. Combined with the definition file, containers only need to install what is absolutely essential to our workflow, sharing everything else with the host OS. This is in contrast to virtual machines, which need to install and run a full OS, requiring more overhead.

Singularity has also been developed with researchers in mind, assuming no administrative privileges and targeting high-performance computing. These reasons have made it ideal for our research. Throughout the course of this paper, we will provide further justification for why we chose both Singularity and Julia as fundamental tools to our work.

2 The Julia Programming Language

Traditionally, high-level dynamic languages have lagged behind lower-level static languages in terms of performance. The emphasis on readability, ease of use, and productivity is believed to come at the cost of run-times and execution speeds. Prototyping is thus done in a high-level language and then fully implemented in a low-level language for speed.