Computational Science in the Battle Against COVID-19—Part II

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The articles in this special issue address the role of computing in battling with the COVID-19 pandemic.

We are currently dealing with a third wave of the pandemic caused by SARS-CoV-2. Cases are spiking in most European countries, Canada, and the United States. The number of reported cases has reached 55 million worldwide, and over 1.3 million people have died.

In the last few months, we could witness the fact that, although natural observations and social experiments are useful, and mathematical modeling is important, computational tools and methodologies are crucial in studying and helping control the spread of the disease. Researchers have developed prediction models to study how to deal with outbreaks using advanced computational science, as reported in this second Special Issue of CISE, with four articles in the forefront of research in computational science applied to the study of COVID-19.

"Supercomputing Pipelines Search for Therapeutics Against COVID-19" by Vermaas *et al.* describes a significant effort to speed up computational drug discovery techniques, as part of the quest for effective treatments for the disease. The idea is to identify promising candidates in a huge database of chemical compounds, preparing a subsequent more thorough, and thus slow and expensive, biomedical examination of these candidates. The drug discovery techniques applied in this article are well known, as they should be: an emergency situation is not the time to perform methodological development. It is the engineering efforts to scale up the drug discovery process with the help of supercomputers that make this work stand out.

The article "Computational Decision Support for the Covid-19 Healthcare Coalition," by Tolk *et al.* outlines the circumstances and the process by which the COVID-19 Healthcare Coalition (C19HCC) was established. The coalition was formed as a coordinated public/private-sector collaboration with the goal of bringing together experts and researchers in a disparate set of fields, ranging from epidemiology and data analytics, to technology and healthcare administration. The authors provide an overview of initial research emerging from the partnership, including efforts to use artificial intelligence and machine learning to predict the spread of SARS-CoV-2 and the use of synthetic populations in computational modeling to better integrate behavioral effects in traditional infectious disease models. Of particular note is the coalition's efforts to bring together and make available a wide array of curated datasets and dashboards to enable future research in pandemics while providing decision-makers with necessary tools for immediate needs.

In "Early COVID-19 Pandemic Modeling: Three Case Studies From Texas, USA," Pierce *et al.* describe the methods and challenges faced in the early days of the pandemic, when data were not available. They used census data to derive key parameters in their models and applied them to a compartmental model. They used a variety of stochastic and deterministic models and calibrated them for uncertainty, calculating the dates for pandemic emergence and hospitalization projections. They show the importance of access to expertise, data, modeling infrastructure, and computational resources to support analysis of the pandemic, in order to give good recommendations to first responders, government agencies, and other stakeholders.

Finally, "Discrete-Time Modeling of COVID-19 Propagation in Argentina With Explicit Delays," shows the work of Castro *et al.* who present a modeling methodology based on discrete-time difference equations

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with explicit delays that allows using daily reported cases reliably. The model takes incubation time, recovery, exposure to the virus, and other timing delays explicitly. The models were validated using publicly available data from public databases in Argentina. The method allows including imported cases and the model parameters are obtained by fitting parameters based on real data. The model provides a new way to predict the evolution of the disease with precision, and it was applied for different cities in Argentina with success.

The Special Issue also includes several department articles related to computational science applied to the study of COVID-19. *Your Homework Assignment* works through a method to build compartmental models and run discrete simulations using a traditional SIR model. The department on *Leadership Computing* discusses the efforts of the COVID-19 High-Performance Computing Consortium for understanding the virus and mechanisms of infection. Two more department articles complete the issue: the *Education* department presents an integrated project in physics, using Raspberry Pi microcontrollers and Python to conduct experiments on capacitor charging and data analysis using open source libraries. Finally, the article on *Diversity and Inclusion* launches from a recent Twitter storm about a NumPy article with 26 male and 0 female authors, to reflect on the context and the forms of dialog that lead to progress.

This is the second Special Issue of CISE focusing on the dissemination of knowledge related to COVID-19. Organizing the Special Issue required extra efforts from authors, as well as reviewers, who had to meet very tight deadlines under the uncertainties of a pandemic. In this volume, we want to acknowledge the hard work by the special issue reviewers, and thank them for their efforts in meeting all the tight deadlines for this issue: Abdolreza Abhari (Ryerson University), Taghreed Altamimi (Carleton University), Joachim Denil (University of Antwerp), Veronica Gil-Costa (National University of San Luis), Dragos Horvath (University of Strasbourg), Rajendra Joshi (Centre for Development of Advanced Computing), Saurabh Mittal (MITRE Corp.), Esteban Mocskos (University of Buenos Aires), Leila Mostaço-Guidolin (Carleton University), Gianluca Palermo (Polytechnic of Milan), David Poza (University of Valladolid), José Luis Risco-Martín (Complutense University of Madrid), Cristina Ruiz-Martín (Carleton University), Mamadou K. Traoré (University of Bordeaux), and Cecilia Zanni-Merk (INSA Rouen).

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