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Computational Science in the Battle Against COVID-19

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■ **IT IS WITH** a sense of urgency that we present this special issue of CiSE on the role of computing in battling the COVID-19 pandemic. In early January 2020, scientists identified SARS-CoV-2 as the cause of a cluster of pneumonia cases in Wuhan City, Hubei, China. The first official death from COVID-19 was reported by China on January 11, and the first death outside of China was reported on February 2nd. The numbers change every day, but as of this writing 24M people worldwide have been infected and over 800 000 of them have died.

As a near-universal scientific instrument, computing is a versatile and effective tool in many aspects of the pandemic response. In this special issue, we have gathered a set of five invited and peer-reviewed papers that we hope will illuminate several of the ways in which computing is playing an important role in response to the devastation of COVID-19.

The first three papers provide a view of computational activities that are aimed at trying to better understand how the virus works, research that contributes to the search for vaccines, and more effective pharmaceutical therapy. Perilla *et al.* discuss the use of molecular simulations to gain

insights into key determinants of infection by characterizing the mechanism by which enveloped viruses, such as SARS-CoV-2, infect cells. Li *et al.* are also involved in the process of understanding infection, using computational simulation to study the features of the interfaces of the so-called spike protein of SARS-CoV-2, which is able to bind to human Angiotensin-Converting Enzyme 2 (ACE2) initializing the entry to the host cell. Amaro *et al.* step back from the details of specific molecular simulations and examine the evolution of the state of practice in biomolecular simulation during the time of COVID-19. Disruptions in established practices include broader adoption of pre-print servers, more open sharing of methods, models, and data, and streamlined processes for accessing critical computing resources quickly. The article discusses the interplay of all of these factors and how they influence biomolecular simulations in the fight against SARS-CoV-2.

Computing also plays a role in the design of more effective near-term therapeutic interventions for patients suffering from the worst effects of the disease. Randles *et al.* describe an airflow simulation developed to help address the need to rapidly expand ventilator capacity for hospitalized patients by splitting ventilators between two or more patients with differing respiratory physiologies.

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Finally, computational models provide important information to health officials and decision-makers as they formulate and implement a public policy response to the pandemic. Reinert *et al.* address the development of a visual analytics application for supporting pandemic preparedness through a tightly coupled epidemiological model and interactive interface.

This special issue also contains several department contributions related to COVID-19. The Visualization Corner in this issue highlights several of the many different visualizations that have played a role in understanding the science and policy surrounding the pandemic. In part one of a two-article series, the Leadership Computing department describes some of the projects that are taking advantage of the largest supercomputing systems in the U.S. computing infrastructure. The Diversity and Inclusion department takes a look at how the pandemic has had a disproportionate impact on members of groups traditionally underrepresented in computing. Finally, in the Education department, the authors explore the impact of the global pandemic on the online course “Problem Solving Using Computational Thinking,” with a particular focus on the topics learners chose for their final projects.

Given the urgency of addressing the pandemic and the role of publications in disseminating knowledge, we felt it was especially important to get this issue out in the same year the pandemic started. Of course, that meant a tremendous effort from authors and reviewers to write and review contributions in an incredibly compressed timeline while the pandemic was still ongoing. We are very grateful for their work. The authors are acknowledged by inclusion of their work in this issue, but we want to make a special gesture to recognize and thank the reviewers for their all-too-often under-appreciated contribution to the health of the academic community: Peter J. Bond (Agency for Science, Technology and Research, A*STAR), Min Chen (Oxford University), Marco De Vivo (Italian Institute of Technology), David Emerson (Daresbury Laboratory, U.K. Science and Technology Facilities Council), Thomas Ertl (Universität Stuttgart), Sergei Grudin (Inria), Michael Hagan (Brandeis University), Yi He (University of New Mexico), Chris North (Virginia Tech), Abhishek Singharoy (Arizona State University), Tamar

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