A look back at 2021

On our one-year anniversary at *Nature Computational Science*, we discuss some of the research that we published over the course of the last year.

One year ago, we launched *Nature Computational Science* with one main goal in mind: providing a platform to publish insightful, inspiring work relevant to the computational science community, as well as to discuss and explore issues of broad interest to this readership. The journal is now celebrating its one-year anniversary, and it has been remarkable to watch this goal become reality. During this first year, our community trusted us to publish many stimulating and noteworthy research works that address challenging scientific problems. Notably, these publications cover a variety of topics, which is also a reflection of the multidisciplinary nature of computational science.

In health sciences, a substantial portion of the work that we published last year was related to the COVID-19 pandemic, which is not necessarily surprising since our research community has been fiercely trying to address the challenges brought by this disease. For instance, Peter V. Coveney et al. sought to examine the reliability of an influential epidemic model by assessing how different sources of uncertainty may affect the quality of that model's predictions. Because epidemic models have been essential for informing governments and public health officials about the pandemic response, this work is important for improving pandemic preparedness now and in the future. Finding potential treatments for COVID-19 is also an important task to help stop the spread of the pandemic, and Josch Konstantin Pauling et al. discussed different computational strategies and research efforts for identifying repurposable drugs for COVID-19. In another line of work, Xavier Rodó et al. studied the association of temperature and humidity with COVID-19, supporting the view that COVID-19 is a seasonal infection: these results can have important implications when designing effective control and prevention measures.

Digital twins have also found their well-deserved space in our journal. A digital twin can be defined as a computational model (or a set of models) that evolves over time to represent the structure and behavior of a corresponding physical asset. There has been a renewed interest in industry, engineering and healthcare in using digital twins throughout the whole asset lifecycle to better guide the design and operational phases using real-time data, but most implementations are custom-based and not generalizable. Karen E. Willcox et al. proposed a foundational mathematical framework to make the implementation of digital twins more uniform and scalable, which has the potential to make this technology more accessible to a wide range of applications. Steven A. Niederer et al. discussed other challenges and opportunities that the community must address in order to further widen the adoption of digital twins, while Neda Mohammadi and John E. Taylor discussed why and how digital twins are promising tools for disaster decision-making in smart cities.

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Other physical science areas were also covered by our journal, some of which we briefly discuss here. Quantum machine learning is an emerging field at the intersection of machine learning and quantum computing, but there are still many questions on whether and how quantum advantage for machine learning can be achieved. Stefan Woerner et al. demonstrated that quantum neural networks can describe more functions than traditional neural networks, suggesting a potentially achievable advantage for quantum machine learning. In materials science, Shyue Ping Ong et al. focused on the prediction of materials' properties by combining data from multiple sources of measurements, achieving high levels of accuracy. In the area of autonomous materials discovery, Andrew I. Cooper et al. introduced a deep-learning tool to automate and facilitate the task of mapping and refining X-ray diffraction patterns to crystal structures, which is traditionally a laborious, manual task, albeit an important one, for chemists and materials scientists. Finally, another topic worth mentioning is automated reaction prediction, where Qiyuan Zhao and Brett M. Savoie proposed a new method for improving the reaction coverage while considerably reducing the associated computational cost.

In the biological sciences, we have published papers covering very distinct topics. For instance, in neuroscience, James C. Knight and Thomas Nowotny proposed an efficient method for large-scale brain simulations using a single GPU workstation, making such simulations more accessible to the community. In structural biology, Xiaoyang Jing and Jinbo Xu focused on protein model refinement, a task that can improve the accuracy of predicted protein structures: they developed a method based on graph neural networks to make the refinement task faster and more accurate.

It goes without saying that this Editorial barely scratches the surface of what we published over the course of the last year. We also compiled a Collection that provides some highlights from 2021, including other areas not mentioned here, such as environmental and urban sciences, and we invite you to check this out.

Of course, our achievements in 2021 would not have been possible without the astonishing support and trust from all of our readers, authors, and reviewers. We want to thank all of you for making *Nature Computational Science* a premier home for computational science research.

Here's to a very productive and successful 2022! ❐

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