Editorial

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A computational quest for a sustainable world

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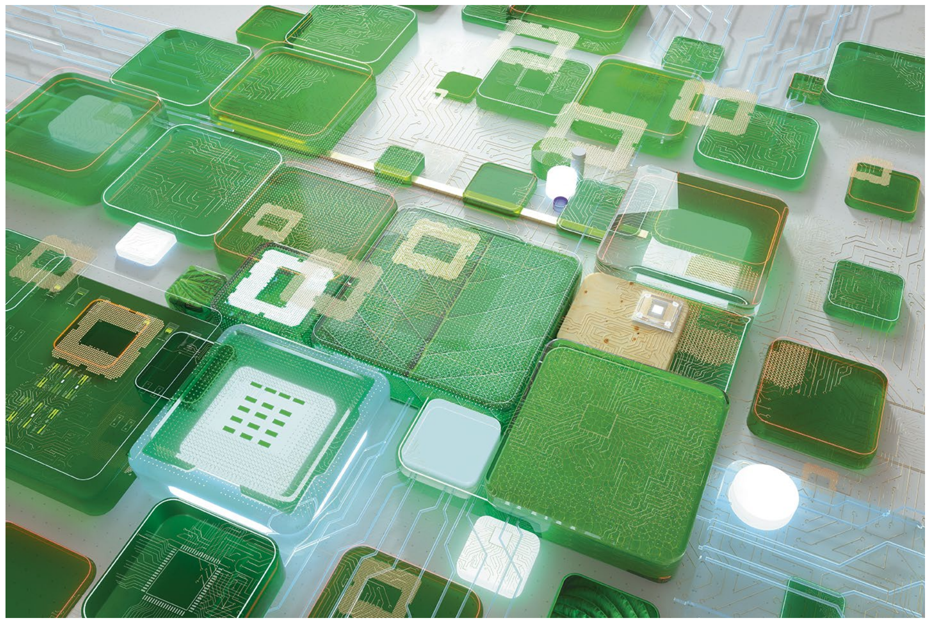
This month's Focus issue highlights ongoing work by computational scientists to help address the Sustainable Development Goals, as well as discusses how the sustainability of computational science itself can be improved.



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In recent years, there have been wide-reaching warnings put forth by international agencies on the potential impact of the ongoing climate and sustainability crisis. These cautions include declining mental health, physical health risks, destabilized economies, and loss of vital biodiversity — to name just a few — mainly as a result of rising temperatures, diminishing air quality, reduced access to quality food and water, changing precipitation patterns, and so on; the list goes on and on. Across different sectors, there is agreement on one thing: urgent action is needed. Accordingly, in 2015 the United Nations (UN) established a set of 17 Sustainable Development Goals (SDGs) that demonstrate the multifaceted nature of the sustainability crisis and that need to be considered both individually and as a whole to help address some of our most pressing challenges. Many scientists are taking the SDGs into consideration to tackle environmental issues, and computational scientists are uniquely poised to contribute to this task, as one can use the ever-growing amount of computing power to draw relevant insights from models and data.

Arguably, one of the most important tasks when addressing sustainability challenges is enacting change at the policy level. A Comment from Edmundo Molina-Perez discusses this point in more detail and emphasizes the value of using decision-support computational tools to empower politicians and the general public with knowledge to make informed decisions about the environment. The value of access to understandable data was echoed in our Q&A with Alexandre Caldas, where he discussed his experience with collecting and meaningfully using diverse environmental data, as well as talked about the UN Environment Programme initiatives to use the available knowledge in order to inform multilateral sustainability policies and develop individualized management strategies for addressing the SDGs. Caldas also noted the disconnect between data and action: "[the] science is clear, but the actual action to do things is very different," he said; this disconnect also applies to investments, as stated by him: "the plans for fossil fuel investments of some of the biggest energy companies in the world are three times larger than they are for renewable energies."

Transitioning from a fossil fuel-based economy to a renewable energy-based one is essential for decreasing carbon emissions and avoiding their harmful side effects, such as ocean acidification, declining air quality, and rising temperatures. This is reiterated in SDG 7 — which aims to ensure access to affordable, reliable, sustainable, and modern energy for all — and SDG 13 — which is concerned with climate change and reducing energy-related carbon dioxide emissions. In a Perspective, Victor Batista and colleagues discuss a strategy for converting solar energy into fuels via artificial photosynthesis. More specifically, the authors discuss the challenges of designing devices to convert carbon dioxide into energy carrier fuels and how we can use computational tools to improve these systems moving forward and eventually realize such a sustainable energy resource. In a Q&A with Y. Shirley Meng, we also spoke about alternative energy resources and the future of battery technology. From Meng's point of view, advancing battery systems will require collaborations between experimentalists and computational scientists, but those collaborations will take intention to cultivate: "we cannot force cross-fertilizations in the short term: it has to happen organically and people need to appreciate each other's languages and cultures and really know each other in order to spark innovation," asserted Meng. Similar to the challenges mentioned by Caldas, Meng discussed the difficulties of data sharing in energy research, particularly between industry and academia, which would, according to her, "require industrial leaders and government bodies to come together to decide what data should be put in the public domain for everyone to study."

In addition to cleaner energy sources, SDG 7 is also concerned with progress in energy efficiency. For computational scientists, the impact on the environment may not be so immediately apparent, but in reality, the energy consumption and efficiency of modern supercomputers has much room for improvement. Loïc Lannelongue and colleagues formulate a set of principles for environmentally sustainable computational science in a Perspective, which calls for researchers to consider the environmental impacts of computational science and to follow the proposed principles in order to maximize the benefit to both humanity and the environment. As we develop new computing platforms — such as quantum computing — questions also arise regarding their energy efficiency. Journalist Sophia Chen investigates in a News Feature to what extent quantum computing can reduce energy usage when compared to classical computing, as well as explores the fact that experts have not yet agreed on a metric to determine the energy consumption of a quantum computer. Moving forward, such a metric will be essential for gauging the level of improvement that quantum computers might provide in the future.

Ensuring that every living creature has access to clean air and water is also an important goal towards a sustainable future, recognized in the SDGs related to health and well-being (SDG 3), clean water and sanitation (SDG 6), and life below water (SDG 14). These goals are featured in Perspectives from the research groups of Jonas Elm and Matthew MacLeod. In the Perspective by Elm and colleagues, a number of data-driven approaches to model atmospheric cluster formation are discussed. Improving our understanding of cluster formation is essential for avoiding their potentially harmful consequences, as aerosol particles influence the global radiation budget, affect cloud properties, and lead to new particle formation driven by atmospheric acids and bases. Meanwhile, MacLeod and colleagues explore in their Perspective how computational tools can be improved to tackle the complex pollution footprint of plastic in environmental water systems. They argue that process-based mass-balance models could provide a platform for improved knowledge about plastic pollution as a function of its properties.

In the same way that life below water must be conserved, it is essential to protect the future of life on land (SDG 15) by, for instance, preserving terrestrial ecosystems and halting biodiversity loss. In a Q&A, Carla Gomes spoke with us about her research on developing diverse and generalizable computational models, including those for strategically planning hydropower dam placement and others that have led to collaborations with the Nature Conservancy to develop and protect waterbird habitats. Gomes's work on computational sustainability strongly links computational science with the UN SDGs: "it's a two-way street: on one hand, we inject computational thinking and methodologies into sustainability challenges, but on the other hand, addressing sustainability problems leads us to novel computational challenges," stated Gomes. This type of mutual enrichment can help to bring together researchers from different fields to tackle some of the most complex environmental problems.

While there are many common themes across the contents of this Focus, the theme that stands out the most is that, moving forward, we must come together with cross-strategy and cross-discipline collaborations if we want to achieve our sustainability goals. It goes without saying that these goals are complex and intertwined, but we cannot let that deter action. In Gomes's words: "'*petit à petit, l'oiseau fait son nid*,' which translates to 'little by little, a bird builds its nest'."

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