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Science and Industry Advance with Computational Modeling

By Daniel Reed

To see a world in a grain of sand,
And a heaven in a wildflower,
Hold infinity in the palm of your hand,
And eternity in an hour.

—William Blake

Computational Science: Illuminating Truth. Without doubt, the scientific method is one of humanity's most powerful and effective tools for understanding the world around us. At its heart, the scientific method relies on testable hypotheses, most often expressed as mathematical models. Indeed, modern science without mathematical models is almost unimaginable. As our models have grown ever more complex and interdisciplinary, so too has their evaluation. In turn, computational science, the evaluation of these complex mathematical models, has emerged as a peer to theory and experiment.

However, that functional definition fails to capture the power and—yes—the beauty of computing in our quest to answer age-old questions about the origins and fate of the universe, the nature of life and its processes, and the fate of this blue orb we call Earth. In a sense, the opening stanza of Blake's *Auguries of Innocence* is a metaphor for our time.

We can see the world in a grain of sand, the silicon from which we build powerful processors, and increasingly sophisticated models hold the promise of in silico biology, an understanding of the life and death of a wildflower from first principles. Our cosmological models—the universe in a box—cannot yet be computed efficiently on a handheld device, but the time is drawing closer. Ah, but eternity in an hour—that perhaps awaits effective quantum computing.

Computing Empowerment. Metaphor aside, computing breathes life into the underlying mathematics of theoretical models, allowing us to understand nuanced predictions and to shape experiments more efficiently. Computing also allows us to capture and analyze the torrent of experimental data being produced by a new generation of scientific instruments and sensors, themselves made possible by advances in computing and microelectronics.

When economics or other constraints preclude experimentation, computing also plays a special and important role by allowing researchers and practitioners to bring theoretical models of phenomena to life. Computational cosmology, which tests competing theories of the universe's origins by computationally evolving cosmological models, is one such example. Given our inability to conduct cosmological experiments (we cannot create variants of the current universe and observe its evolution), computational simulation is the only feasible way to conduct experiments.

Computing also enables researchers to evaluate larger or more complex models and to manage larger volumes of data than would be possible otherwise. Although this may seem prosaic, the practical difference between obtaining results in hours, rather than weeks or years, is substantial—it qualitatively changes the range of studies that can be conducted. For example, climate change studies, which simulate thousands of Earth years, are feasible only if the simulation time for a year of climate is a few hours. Moreover, conducting parameter studies (e.g., to assess sensitivity to different conditions, such as the rate of fluorocarbon or CO_2 emissions) is possible only if the time required for each simulation is small.

Finally, computing allows us to couple models to understand the interplay of processes across interdisciplinary boundaries. Understanding the environmental and biological bases of respiratory disease or biological attack requires coupling of fluid dynamics models of airflow and inhalants, whether smoke, allergens, or pathogens, materials models of surface properties and interactions, biophysics models of cilia and their movements for ejecting foreign materials, and deep biological models of the genetic susceptibility to disease. The complexity of these interdisciplinary models is such that they can be evaluated only via computers, most often very high-performance computers.

The Intellectual Amplifier. The breadth of these examples highlights a unique aspect of computational modeling that distinguishes it from other scientific instruments—its universality as an intellectual amplifier. Powerful new telescopes advance astronomy, but not materials science. Powerful new particle accelerators advance high-energy physics, but not genetics. In contrast, computing and computational models advance all of science and engineering, because all disciplines benefit from high-resolution model predictions, theoretical validations, and experimental data analysis. As new scientific discoveries increasingly lie at the interstices of traditional disciplines, computing and computational models via applied mathematics are the enabler of research integration.

As applied mathematicians and computational and computer scientists, we are on the vanguard of a new future, where computing becomes fully synonymous with scientific discovery. The universe in a grain of sand is here.

Daniel Reed is Microsoft's Scalable and Multicore Computing Strategist and a member of the President's Council of Advisors on Science and Technology (PCAST). He also chairs the board of directors of the Computing Research Association (CRA). The opinions expressed above are his, not necessarily those of Microsoft or the federal government. Readers can contact him at Daniel.Reed@microsoft.com or his blog at www.hpcdan.org.