Supercomputing has become ubiquitous in scientific research—nearly every area of science and engineering is strongly positively impacted by computational modeling and data analysis. Supercomputing affects our everyday life in many ways, for example, by providing reliable weather prediction and efficient airplane design. Recently, the Nobel Prize in Physics was awarded for the Laser Interferometer Gravitational-Wave Observatory’s (LIGO’s) direct detection of gravitational waves from a binary black hole system, one of the most profound discoveries in astrophysics. These gravitational waves were predicted by Einstein himself more than a century ago (!) but had not been found previously. This discovery was as much a computational science success as an experimental one, because “template” signals from accurate computational models are crucial for performing signal searches in the very noisy LIGO data stream.

Broader access to supercomputing resources is one of the major reasons that scientific computing has become so pervasive and impactful in scientific and engineering applications. Beowulf cluster computing allows one to string together low-cost commodity parts and build a supercomputing class system very affordably. In addition, major R&D investments by the large consumer electronics industry have highly subsidized significant advances in supercomputing. For example, the quantum jump to petascale supercomputing came as a result of Sony’s investments in the development of the Cell processor for the PlayStation 3 gaming console. Similarly, the adoption of GPU-accelerators in supercomputers in recent years is a result of the rapid increase in GPU performance that, in turn, was driven entirely by the demands of the video-gaming industry. Beyond the issue of cost and hardware innovations, advances on the software and applications side are also making supercomputing far more affordable and accessible today. In addition, federal funding agencies like the US’s National Science Foundation (NSF) have made major investments toward supporting scientific-computing-related educational activities that are beginning to pay off. We are truly living in an era of supercomputing democratization.

As directors of the University of Massachusetts, Dartmouth’s Center for Scientific Computing and Visualization Research—which now has more than 30 faculty engaged in very diverse areas of science and engineering—we’ve witnessed the tremendous growth of this discipline over the past decade. Our faculty affiliates come from across disciplines in engineering, mathematics, physics, chemistry, biology, and fisheries. Scientific computing unites us and allows us to transcend disciplinary boundaries.
Given the recent advances in supercomputing and an increased awareness of the field’s importance, we thought this was the perfect time for CiSE to publish a dedicated issue on the scientific advances enabled by supercomputing. We were particularly interested in reviewing articles from several different research fields, especially those reporting on significant scientific advances. We ultimately selected five excellent articles, introduced briefly below, which offer a taste of the range of advances enabled by supercomputing. These articles feature applications in astrophysics, engine simulations, and drug discovery while highlighting an array of supercomputing tools, from fundamental algorithms to innovative hardware and cloud computing.

In “A Note on QR-Based Model Reduction: Algorithm, Software, and Gravitational Wave Applications,” Harbir Antil, Dangxing Chen, and Scott Field describe a low-rank matrix approximation method that exhibits excellent parallel scaling performance—well over 30,000 cores! This article is an excellent example of fundamental advances in supercomputing algorithms that are useful for a variety of applications. The method shows great promise not only for parameter inferences in the context of gravitational-wave-related data analysis, but could also be applicable to many other science and engineering areas.

“Glimpses of Space-Time beyond the Singularities Using Supercomputers” by Parampreet Singh is a fascinating article about how supercomputing is allowing us to unlock some of the biggest secrets of our universe, helping us develop an understanding of the physical singularities that lie at the heart of black holes and the big bang itself. Such work might allow us to answer questions about the origin of the big bang and thus yield an answer to the deepest question of all.

“An Asynchronous Two-Level Checkpointing Method to Solve Adjoint Problems on Hierarchical Memory Spaces” is a more technical article that presents a novel data-movement strategy to address the adjoint problems that are common in many time-dependent partial differential equation systems. Authors Debanjan Datta, David Appelhans, Constantinos Evangelinos, and Kirk Jordan use bleeding-edge supercomputing hardware for their numerical results, demonstrating that they can run much larger simulations faster than with current approaches. This article provides a glimpse into the future promise of scientific computing.

“Advanced Computational Simulations of Surface Impingement of a Train of Ethanol Drops: A Pathway to Developing Spray-Wall Interaction Submodels,” by David Markt, Ashish Pathak, and Mehdi Raessi, demonstrates how supercomputers can be used to generate very-high-quality datasets for the unprecedented micron-scale submodels of spray-wall interactions, meant for full engine simulations. This is a fascinating application of supercomputing to the real-world challenge of improving engine design.

Lastly, “Leveraging Cloud Computing for In-Silico Drug Design Using the Quantum Molecular Design (QMD) Framework” describes a very important application of supercomputing to pharmaceutical drug design. In this article, authors Shahar Keinan, Elizabeth Hatcher Frush, and William Shipman utilize cloud resources for their work, thereby touching on another important aspect of supercomputing today.

We extend our thanks to all of the authors for their excellent submissions and to the highly attentive and professional CiSE staff for making the process of assembling this special issue very straightforward. We hope you enjoy reading this issue as much as we enjoyed editing it! Please feel free to drop us a line using the contact information provided below.

ABOUT THE AUTHORS

Sigal Gottlieb is a professor of mathematics and co-director of the Center for Scientific Computing and Visualization Research at the University of Massachusetts, Dartmouth. Contact her at sgottlieb@umassd.edu.

Gaurav Khanna is a professor of physics and co-director of the Center for Scientific Computing and Visualization Research at the University of Massachusetts, Dartmouth. Contact him at gkhanna@umassd.edu.