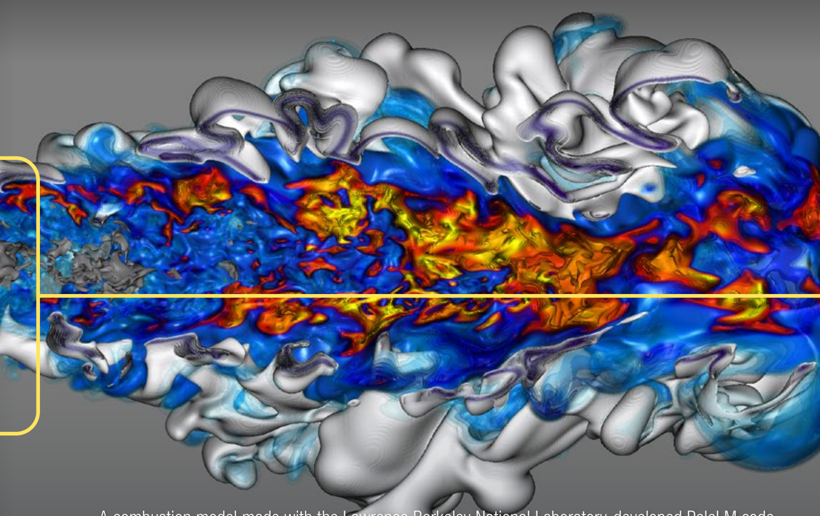
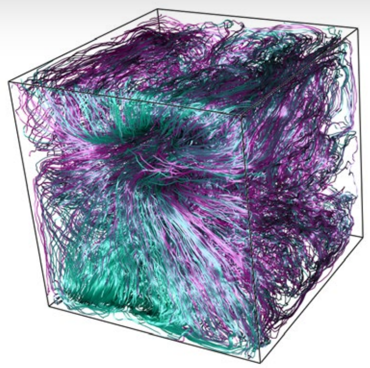
A REVOLUTION IN MODELING AND SIMULATION

Computational Science Fuels Discovery



A combustion model made with the Lawrence Berkeley National Laboratory-developed PeleLM code. *Credit: D. Dalakoti and E. Hawkes/University of New South Wales, M. Day and J. Bell /Berkeley Lab.*

Unprecedented advances in computing power over the past few decades have supported a major revolution in computational modeling and simulation. This new field, computational science, combines mathematics, software and computer science with high-performance computing (HPC) to solve some of the nation's most pressing scientific and technical challenges. The Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program invested in the key computer hardware that facilitated this progress. However, these new scientific and engineering discoveries would not have happened without the significant advances in mathematical models, methods, algorithms and software technologies that allowed scientists and engineers to take full advantage of the hardware.



A flow-transport simulation based on the fluid dynamics code Nek5000. *Credit: J. Zhang, F. Hong and X. Yuan/Peking University, A. Obabko, H. Guo and T. Peterka/Argonne National Laboratory.*

INNOVATIONS

PROGRESS OVER DECADES

Scientific computing traces its roots to DOE's predecessor and has evolved over the decades since, from interdisciplinary programs and leadership-class computing facilities to the Exascale Computing Project.

- **1950s:** DOE's forerunner, the Atomic Energy Commission, founded DOE's Mathematics Program—the early predecessor of ASCR.
- **By the 1970s:** many DOE national laboratories had built facilities with leading-edge computer hardware.
- **Early 1990s:** DOE and ASCR created the DOE Computational Science Graduate Fellowship to train an interdisciplinary workforce.
- **Early 2000s:** DOE and ASCR launched the Scientific Discovery through Advanced Computing (SciDAC) program, which brings together interdisciplinary teams to support key advances in science and engineering.
- **Today:** DOE's ongoing Exascale Computing Project will provide both the next generation of HPC hardware and a suite of scientific and engineering application codes to support future discovery and innovation.

IMPACT

SCIENTIFIC ADVANCES

Virtually every discipline in science and engineering has benefited from DOE's sustained investment in computing.

- Advanced computational chemistry software can predict molecular properties without experiments.
- Powerful fusion energy simulations predict reactors' complex behavior.
- Astrophysical codes explain supernova explosions.
- Mathematical and computational advances underpin DOE's state-of-the-art global climate modeling system.
- Advanced simulation methods can calculate all possible nuclear isotopes.

TAKEAWAY

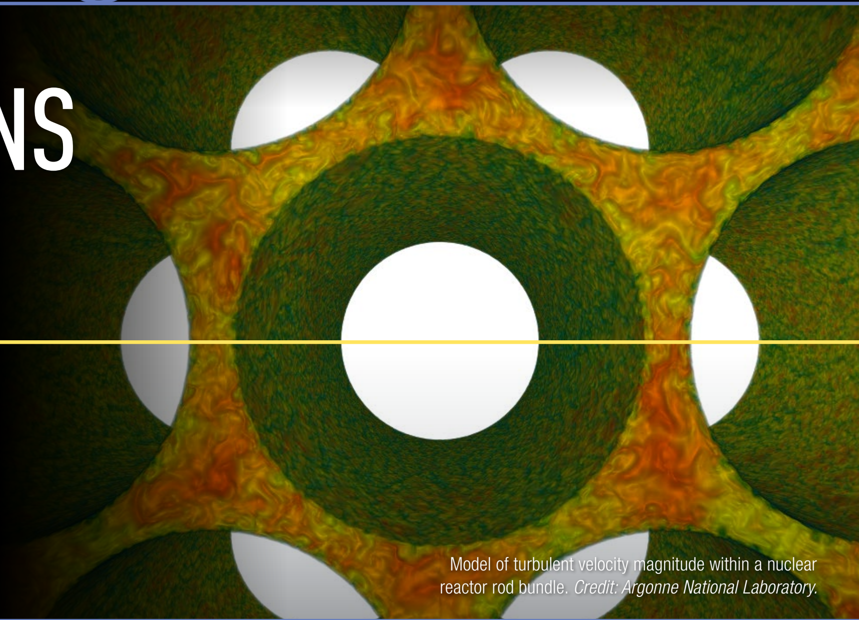
AN INDISPENSABLE TOOL FOR DISCOVERY

ASCR's decades of investments in mathematical and computing research and computing platforms have allowed computational science to emerge as a uniquely powerful discovery pathway in science and engineering.

Content provided by Department of Energy multiprogram laboratory researchers. Prepared by the Krell Institute for the ASCAC Subcommittee on the 40-year History of ASCR.

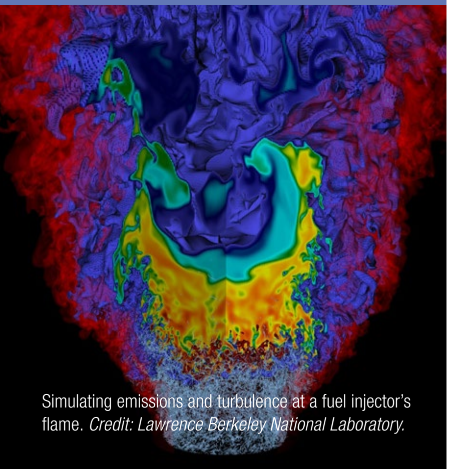
APPLYING EQUATIONS TO COMPLEX PROBLEMS

Building Models with Mathematics



Model of turbulent velocity magnitude within a nuclear reactor rod bundle. *Credit: Argonne National Laboratory.*

Scientists describe the world using mathematics. Equations for phenomena such as electromagnetism and fluid mechanics, for example, were derived in the 19th century. Although those equations help researchers understand natural phenomena, they rarely can be solved directly. In the early 1950s, mathematician John von Neumann recognized that digital computers programmed to translate equations into digestible mathematical problems could solve these scientific puzzles. To realize this vision, the Department of Energy's (DOE's) forerunner created the Applied Mathematical Sciences program.



Simulating emissions and turbulence at a fuel injector's flame. *Credit: Lawrence Berkeley National Laboratory.*

INNOVATIONS

NEW APPROACHES TO COMPLEX PROBLEMS

Scientists funded by the Advanced Scientific Computing Research (ASCR) program and its predecessors created methods for representing the mathematics of physical systems on a computer. This work has addressed several important issues, from representing key science features to creating predictable software. These methods have led to accurate and efficient simulations of complex phenomena.

- During World War II, researchers wanted to model shock waves to understand the dynamics of explosions. Simulating those fluid dynamics phenomena has led to efficient and accurate methods for computing more general high-speed fluid flows.
- Complex chemical reactions and other systems can involve processes that occur on both fast and slow time scales. Understanding the mathematics of those systems has led to various methods for determining when it is possible to skip over the fast time scales in computational simulations.

IMPACT

POWERFUL TOOLS FOR SCIENCE AND INDUSTRY

Mathematical and computational methods developed with ASCR's support are now used for modeling and simulation across numerous areas of science and technology. Modern computational science would not be possible without these foundational mathematical advances.

- Fluid dynamics codes are used to model astrophysics, aerodynamics, bioengineering and combustion and to design nuclear reactors.
- Industry has applied these tools to simulate chemical reactors, semiconductor etching and image processing.

TAKEAWAY

MATH UNDERLIES COMPUTING ADVANCES

Long-term investments in developing mathematical methods for computer simulations have paid off, both in solving the original DOE science problems that motivated them and in providing solutions for many other domains.

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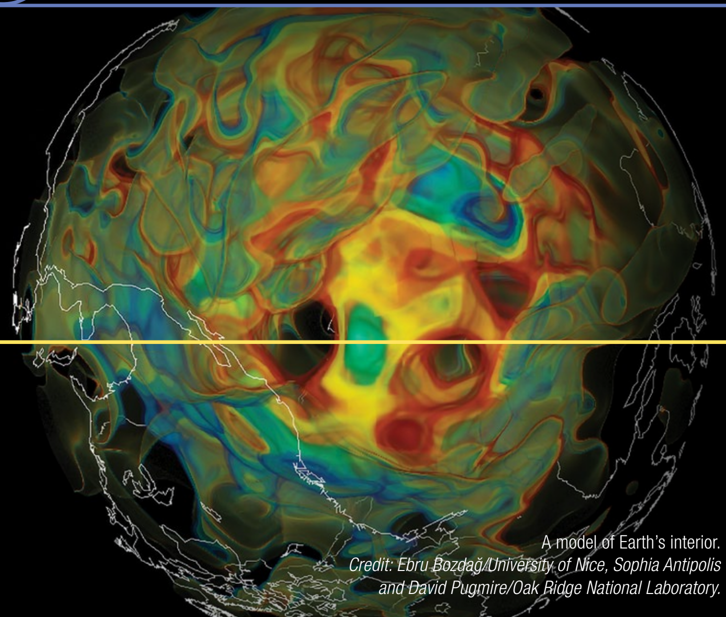
UNCERTAINTY QUANTIFICATION

Building in Probability to Interpret Simulations



A model of Earth's interior.
Credit: Ebru Bozdağ/University of Nice, Sophia Antipolis and David Pugmire/Oak Ridge National Laboratory.

Science relies on experiments and observation. Yet traditional physical experiments can be difficult, costly or even impossible—we can't, for example, easily poke around inside nuclear reactors, lasers or stars. Such difficulties lead to experimental uncertainty. Computer simulations are increasingly used to fill the gap, but they're also inherently inexact. Uncertainties in computer simulations arise from several sources, from imprecise knowledge of a system's properties and external conditions' natural variability to a system's unknown initial state. To be useful, any simulation-based design and scientific result must account for uncertainties. To address this need, the Department of Energy's Office of Advanced Scientific Computing Research (ASCR) has played a central role in building a scientific discipline now known as uncertainty quantification (UQ).

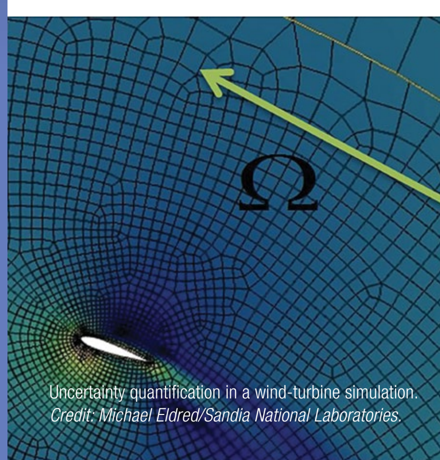
Since the early 2000s ASCR has invested in UQ basic research and applications. All mission-critical simulations—economic, environmental, national security and more—now include UQ, allowing researchers to consider factors such as outcome probabilities, input-condition sensitivity and simulation-failure likelihood. Notably, UQ is an essential part of all computations used for high-consequence decisions in many applications: designing microbes for biofuels, forecasting environmental changes, developing fusion-power technology, buttressing the nation's power grid and much more.

INNOVATIONS

UNCERTAINTY QUANTIFIED

ASCR has supported basic research and the development of tools that allow scientists to understand, design and optimize complex systems while quantifying confidence and assessing uncertainty.

- Development of foundational mathematical methods for UQ.
- Broad deployment of computationally efficient UQ tools.
- Fundamental shift in how modeling and simulation is used to inform critical decisions.



Uncertainty quantification in a wind-turbine simulation.
Credit: Michael Eldred/Sandia National Laboratories.

IMPACT

A RISE IN PREDICTIVE RELIABILITY

Because of UQ, computational scientists now perform simulations with quantified reliability, a perspective that shapes a variety of disciplines.

- The oil industry increasingly uses UQ to discover resources and manage reservoirs.
- UQ is critical to the simulation-based design process for nearly every aircraft and automobile.
- The pharmaceutical industry is adopting UQ for drug design, and the medical community is using these tools to support surgical decisions.
- UQ is a central element of DOE's stockpile stewardship mission.

TAKEAWAY

ASCR HAS LED THE WAY IN UQ

As computer simulations have improved, quantifying their uncertainty has become critical for assessing the reliability of predictions. ASCR has played a formative role in uncertainty quantification. UQ is now a central tenet of computational science, shaping critical decision-making in numerous fields.

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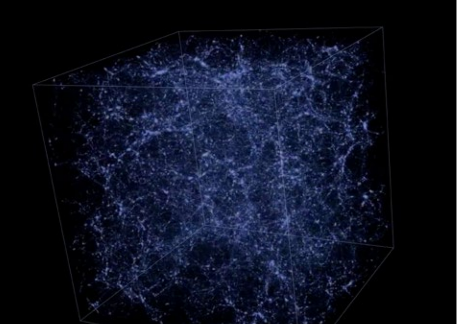
MOVING BIG DATA

DOE's Ultra-Fast Communication Network User Facility Supports Global Science

ESnet moves big data at blistering speeds. *Credit: ESnet.*

Computer networks are 10 million times faster than they were 40 years ago, rocketing from a meager 56 kilobits per second in 1980 to more than 100 gigabits per second today. The Department of Energy's (DOE's) networking innovations have driven key improvements and provided scientists and engineers with extremely high-speed connections to support science at every corner of the United States and abroad. Today the Energy Sciences Network (ESnet), a state-of-the-art user facility supported by DOE's Office of Advanced Scientific Computing Research (ASCR), moves massive quantities of data to enable ground-breaking science in many disciplines such as physics, fusion energy, biology, and the environmental and energy sciences.



Visualizing the universe's evolution. *Credit: ESnet.*

INNOVATIONS

INFRASTRUCTURE THAT KEEPS DATA MOVING

DOE innovations drove the establishment of ESnet, the world's fastest network dedicated to science.

- Network protocols developed by ASCR researchers overcame early internet design flaws that caused data traffic jams. The algorithms they devised remain the foundation of today's tools for avoiding internet congestion.
- ASCR researchers developed circuit reservation mechanisms that allow researchers to obtain guaranteed bandwidth at scheduled times. This ensures they can move massive, time-sensitive data sets efficiently to collaborators thousands of kilometers apart.
- The ASCR-funded Science DMZ architecture underpins fast, secure research infrastructure at the U.S. national laboratories, universities and beyond.

IMPACT

LARGE-SCALE COLLABORATION AND DISCOVERY

Sustained ESnet upgrades over four decades have continued to push the boundaries of performance, reliability and programmability.

- The rapid movement of vast quantities of data over ESnet was a key contributor to the Nobel Prize-winning discovery of the Higgs boson in 2012.
- Today ESnet moves more than four petabytes of data—the equivalent of a million high-definition movies—across the United States and internationally every day. That's more than an exabyte each year.
- ESnet connects with more than 150 research and education networks and cloud providers, placing DOE laboratories at the center of international science.

TAKEAWAY

ESNET KEEPS U.S. SCIENCE ON THE LEADING EDGE

The rapid communication network established and operated by DOE is essential to scientific discovery. Innovations by ASCR-funded scientists have kept DOE at the leading edge of networking for more than four decades, giving DOE a significant edge in modern scientific discovery.

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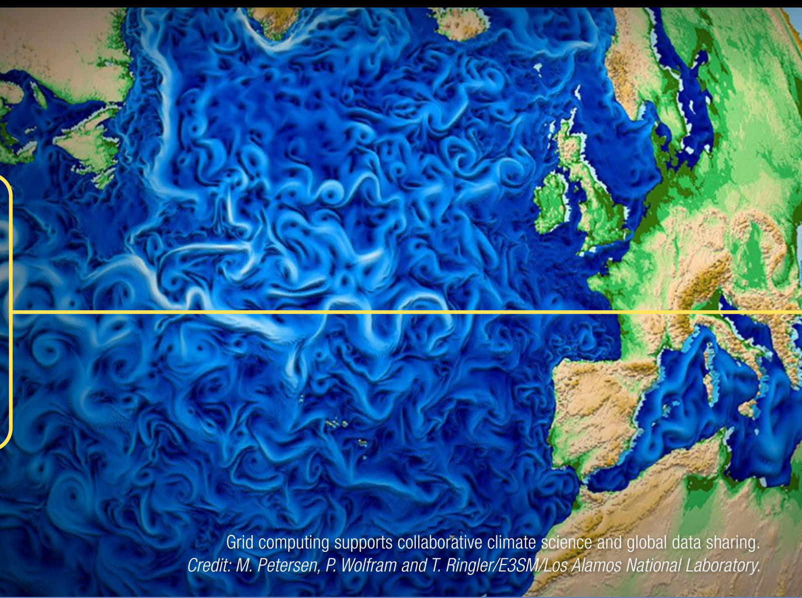
GRID COMPUTING FOR HIGH-SPEED COLLABORATION

Secure, Reliable Data-Sharing Connects Far-Flung Scientists



Grid computing supports collaborative climate science and global data sharing.
Credit: M. Petersen, P. Wolfram and T. Ringler/E3SM/Los Alamos National Laboratory.

Modern science's large scale and rapid pace require researchers to engage instantaneously with remote colleagues, supercomputers, scientific facilities and databases, regardless of location. But innovative software is needed to stitch people, computers and networks into a boundary-free collaboration fabric, a grid that helps scientists reliably and securely find needed data, dispatch data to supercomputers for analysis and share results with collaborators—all with the click of a button. For decades DOE's Office of Advanced Scientific Computing Research (ASCR) has supported methods and software needed for data-intensive networked collaboration, establishing DOE laboratories as the global leader in grid computing.

Collaborating through DOE's Access Grid.
Credit: Argonne National Laboratory.

INNOVATIONS

SOFTWARE KNITS TOGETHER THE GRID'S FABRIC

ASCR has supported novel software that facilitates grid computing: data communication and collaboration among thousands of institutions.

- The GridFTP protocol and Globus software allow rapid, reliable and secure data exchange and sharing among research institutions.
- Universal trust fabric connects people, data and computers worldwide and protects sensitive and proprietary information.
- Programmatic interfaces allow easy automation of distributed data sharing, remote instrumentation and collaboration applications—key to accelerating research.

IMPACT

GRID COMPUTING BACKS IMPORTANT SCIENCE

ASCR-supported software underlies groundbreaking research findings.

- Grid computing has enabled the Nobel-prize-winning discoveries of the Higgs boson and gravitational waves.
- The Earth System Grid Federation supports global sharing of large climate data sets used in the Intergovernmental Panel on Climate Change assessments.
- Collaboration software connects thousands of scientists and engineers to remote DOE facilities, driving discoveries in materials, energy, environmental science, life sciences and other disciplines.

TAKEAWAY

UNIVERSAL CONNECTIVITY FUELS DISCOVERY

ASCR's investment in fundamental software research to reinvent online, data-driven discovery has given DOE a significant edge in modern science.

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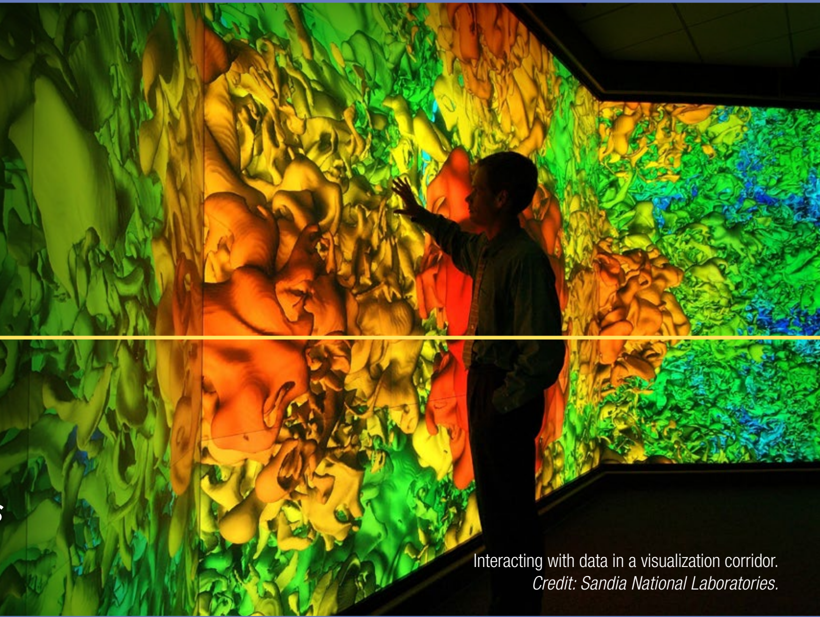
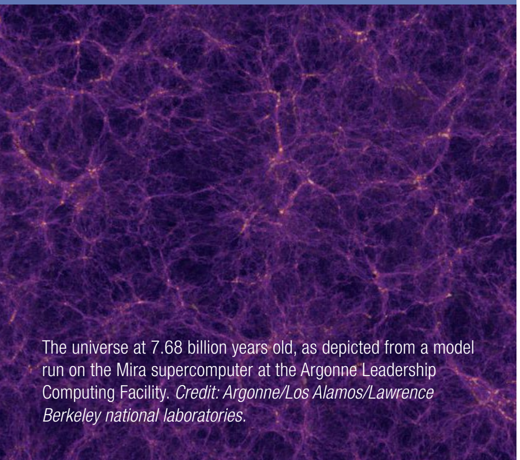
MAKING SENSE OF BIG DATA

Developing Data Analysis and Visualization Tools



Interacting with data in a visualization corridor. *Credit: Sandia National Laboratories.*

Because large computational simulations produce enormous datasets, extracting and highlighting salient information presents significant challenges. As data volumes continue to grow, researchers have needed to harness many processors and develop parallel methods to store and sift through results for timely analysis. In addition, researchers have developed functional and adaptive visualization software and hardware to help them understand and interact with simulation results. In the past two decades, the Advanced Scientific Computing Research (ASCR) program has funded state-of-the-art tools for grappling with these challenges, including the development of large-scale data analysis and visualization software and specialized display devices.



The universe at 7.68 billion years old, as depicted from a model run on the Mira supercomputer at the Argonne Leadership Computing Facility. *Credit: Argonne/Los Alamos/Lawrence Berkeley national laboratories.*

INNOVATIONS

OPEN-SOURCE SOFTWARE AND HARDWARE ADVANCES

Twenty years ago, ASCR began funding research on data analysis and visualization, leading to solutions that accelerate research in a variety of fields.

- Open-source scientific data analysis and visualization software such as ParaView and VisIt.
- Specialized display technologies, such as the Cave Automatic Virtual Environment, an immersive virtual reality space that allows scientists to interact with simulation data within a room-like area.
- Indexing technologies, such as FastBit, find important results in large data volumes. Compression methods reduce the overall footprint of scientific data. And online analysis methods eliminate data-storage-and-retrieval time.
- New workflows that analyze data as they are produced rather than archiving information for later analysis. These methods optimize DOE user-facility collaborations and allow real-time data analysis and on-the-fly experimental adaptation.

IMPACT

INSIGHTS AND ENHANCED PRODUCTIVITY

ASCR's investments in data analysis and visualization have contributed to significant scientific advances.

- Scientific insights in diverse research areas, from drug discovery to combustion to cosmology.
- Enhanced productivity on DOE's experimental user facilities.
- Scientific discovery through machine learning.

TAKEAWAY

A NEW TOOL FOR DISCOVERY

ASCR's investments in large-scale data analysis and visualization have advanced knowledge across a broad range of scientific disciplines, leading to data-driven discoveries.

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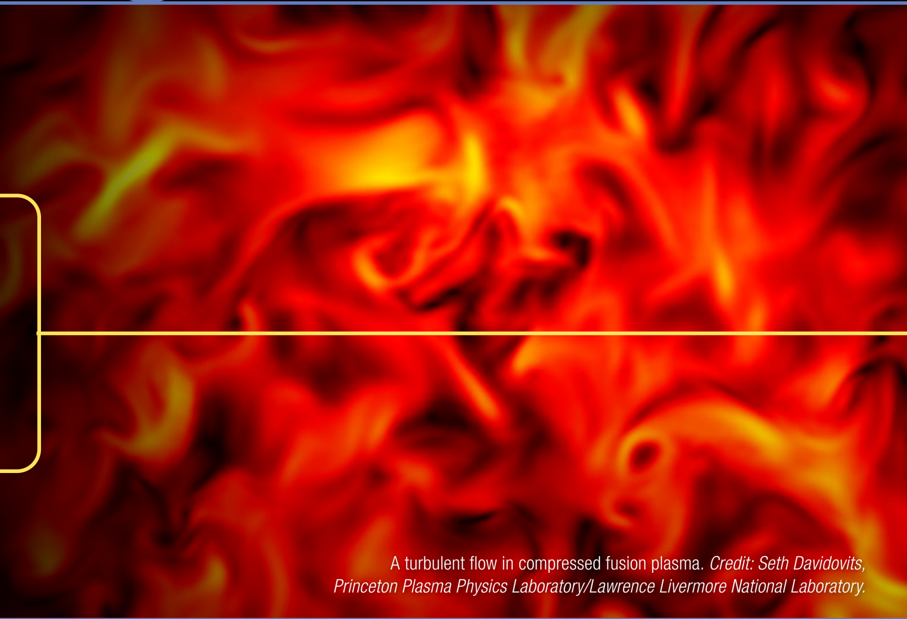
OVERCOMING SCALING CHALLENGES

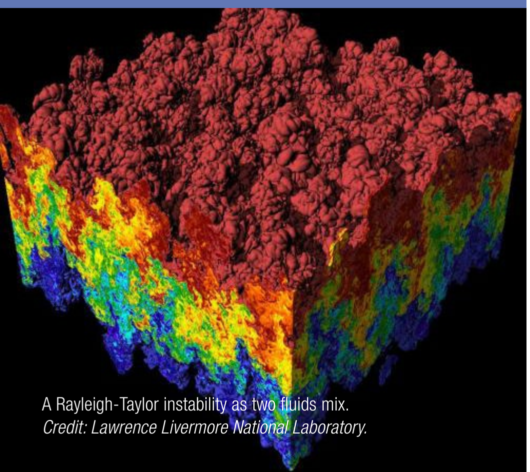
Massively Parallel Processing Systems Boost Computer Power and Speed



A turbulent flow in compressed fusion plasma. *Credit: Seth Davidovits, Princeton Plasma Physics Laboratory/Lawrence Livermore National Laboratory.*

Nearly four decades ago, Department of Energy (DOE) laboratories recognized that the prevailing vector supercomputing technology would need to be replaced with systems that used many smaller microprocessors to support the ever-growing need for computational power and speed. Today these massively parallel processing (MPP) systems have become the dominant approach for building the most powerful computing systems in the world.

That successful shift was built directly on coordinated R&D investments from the Advanced Scientific Computing Research (ASCR) program. Before MPP systems could be used for scientific discovery, researchers needed to address scaling challenges at every level, from building the communication fabric needed to connect thousands of microprocessors to developing scientific applications.



A Rayleigh-Taylor instability as two fluids mix. *Credit: Lawrence Livermore National Laboratory.*

INNOVATIONS

MPI, PGAS, UPC AND SOFTWARE INFRASTRUCTURE

ASCR's R&D investments in programming models and systems, system software, and communication libraries were critical to the large-scale use of MPP in science.

- ASCR support led to several programming standards, including MPI (message passing interface), PGAS (partitioned global address space) and UPC (unified parallel C) that enabled applications to be developed for MPP systems.
- ASCR's further support of system software, message-passing libraries and underlying algorithms ensured that these applications could effectively harness MPP systems and helped researchers produce software that was portable across different systems. These technologies, adopted by industry, have formed HPC's ecosystem over the past three decades.

IMPACT

ASCR HAS CREATED AN MPP ECOSYSTEM

ASCR's investments combined with DOE's R&D investments in applications through the Scientific Discovery through Advanced Computing (SciDAC) program and partnerships with industry vendors have boosted computational capabilities for science.

- When acquiring new supercomputers, DOE viewed industry vendors as partners.
- Improvements in MPP systems support science advances, which, in turn, lead to further advances in MPP and a larger industry market for MPP systems, paving the way for tomorrow's computers and assuring U.S. leadership in the field.

TAKEAWAY

A MASSIVE RETURN ON COMPUTING INVESTMENT

ASCR R&D investments in scalable programming models, system software and communication libraries laid the foundation for today's key computational science applications.

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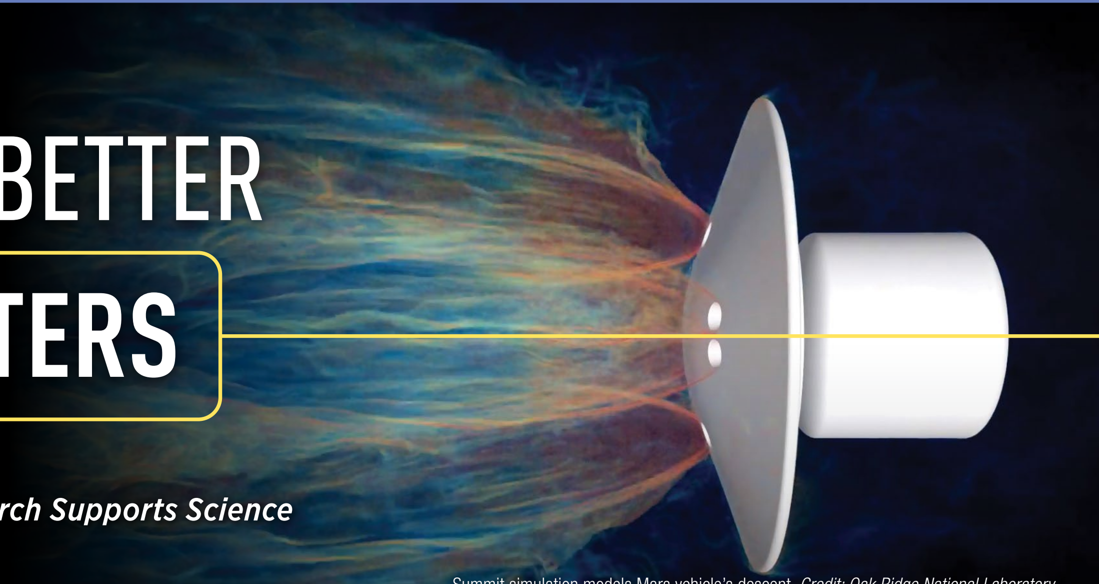
BUILDING BETTER COMPUTERS

Computer Architecture Research Supports Science



Summit simulation models Mars vehicle's descent. *Credit: Oak Ridge National Laboratory.*

The Department of Energy (DOE) has fostered a decades-long collaboration between its Advanced Scientific Computing Research (ASCR) program and the U.S. computer industry. As Moore's Law reaches its limits, that approach continues to shape high-performance computing (HPC) today. Researchers can no longer rely on packing more processors onto ever smaller silicon chips. Instead, they must make dramatic changes to computer architectures to continue to boost computational performance. ASCR researchers are working closely with industry partners to ensure that future machines will meet DOE's needs.

Credit: Oak Ridge National Laboratory.

INNOVATIONS

PARTNERSHIPS WITH INDUSTRY SHAPE ADVANCED COMPUTING

Partnerships between ASCR-funded researchers and industry have long been central to HPC. For example, in the 1980s and early 1990s ASCR-funded researchers pioneered and drove the transition to massively parallel computers through close collaborations with industry.

- DOE purchased cutting-edge machines to support innovative scientific research.
- ASCR has helped shape the direction of high-performance computing through investments in architecture research, systems software and applications.
- The collaboration in parallel computing also benefitted the U.S. computer industry, which used those valuable lessons to produce leading hardware and software for the commercial marketplace.

IMPACT

DESIGNING HARDWARE, ALGORITHMS AND SOFTWARE SIMULTANEOUSLY

ASCR researchers have pioneered co-design, an approach that weighs tradeoffs among hardware, software and algorithms to find the best computing solutions.

- This co-design approach led to today's fastest supercomputers, such as Summit at the Oak Ridge Leadership Computing Facility. Summit has reached a peak performance of 200 petaflops (quadrillion scientific calculations per second) through the combination of CPUs with graphics processing units.
- ASCR's collaboration with the DOE National Nuclear Security Administration's Advanced Scientific Computing program on the Exascale Computing Initiative is ensuring that DOE supercomputers continue to lead the world as tools for scientific discovery while positioning U.S. computer vendors to succeed commercially.

TAKEAWAY

NAVIGATING A HETEROGENEOUS FUTURE

ASCR's collaborations with industry have guided the design of novel computer architectures and are supporting the development of tomorrow's exascale supercomputers, capable of a billion-billion calculations per second.

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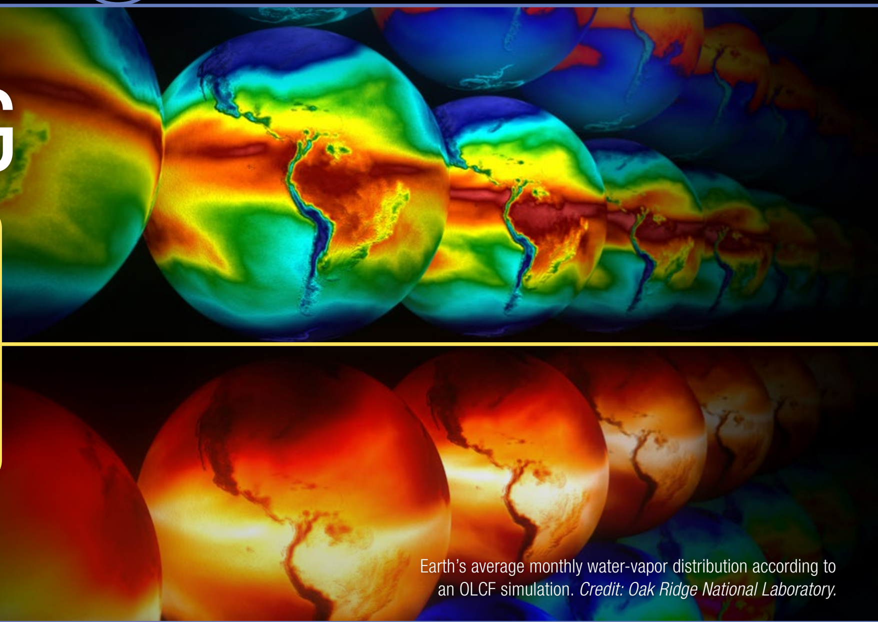
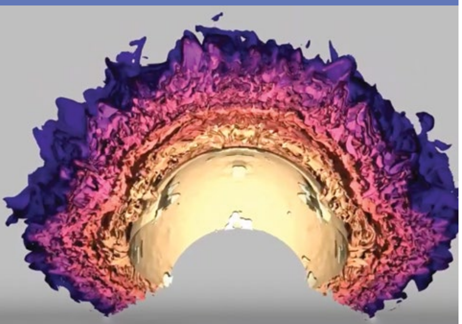
WORLD-LEADING COMPUTING FACILITIES

Computational Science Fuels Discovery



Earth's average monthly water-vapor distribution according to an OLCF simulation. *Credit: Oak Ridge National Laboratory.*

Solving the world's most challenging scientific and societal problems requires the world's most powerful supercomputers and data analysis facilities. The Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program anticipated this need decades ago and devised a first-of-its-kind nationwide infrastructure of supercomputing centers connecting DOE scientists and thousands of university and industry researchers via the world's fastest and most advanced scientific network. Scientists from across the U.S. and the world use these facilities, located at Argonne, Lawrence Berkeley and Oak Ridge national laboratories, to tackle the world's toughest scientific and technical challenges.



Extreme turbulence from a hydrodynamic simulation of a massive star. *Credit: University of California, Santa Barbara and Joseph A. Insley/ALCF.*

INNOVATIONS

A WORLD-CLASS ENSEMBLE OF ADVANCED MACHINERY AND EXPERTISE

ASCR's HPC facilities provide unique resources and support for cutting-edge research—at government labs, universities and in industry—that couldn't be done any other way.

- The leadership computing facilities at Argonne and Oak Ridge national laboratories (ALCF and OLCF) provide the world's most powerful supercomputers to researchers on a competitive basis for addressing grand challenges in science, health and technology.
- Located at Lawrence Berkeley National Laboratory, the National Energy Research Scientific Computing Center (NERSC) provides world-class resources to support the mission priorities of the six DOE Office of Science program offices.
- ALCF, OLCF and NERSC support users with scalable workflows and software for data-intensive computing. All three facilities are evaluating and implementing machine learning and artificial intelligence as powerful computational tools for future discoveries.

IMPACT

FACILITIES DRIVE SCIENTIFIC AND TECHNOLOGICAL DEVELOPMENT

Virtually every discipline in science and engineering has benefited from DOE's sustained investment in computing.

- DOE's HPC national user facilities have hosted thousands of researchers from all 50 states and many countries and provide a training ground for tomorrow's computational science workforce.
- By leveraging these facilities, U.S. scientists lead computational science research, producing thousands of high-impact research publications each year.
- Groundbreaking computing and data systems installed at ASCR's HPC facilities drive technological innovation in industry, paving the way for tomorrow's computers and assuring U.S. leadership in the field.

TAKEAWAY

HPC FACILITIES HAVE LEFT AN INDELIBLE MARK ON SCIENCE

DOE's supercomputing facilities are a unique national resource in support of scientific discovery.

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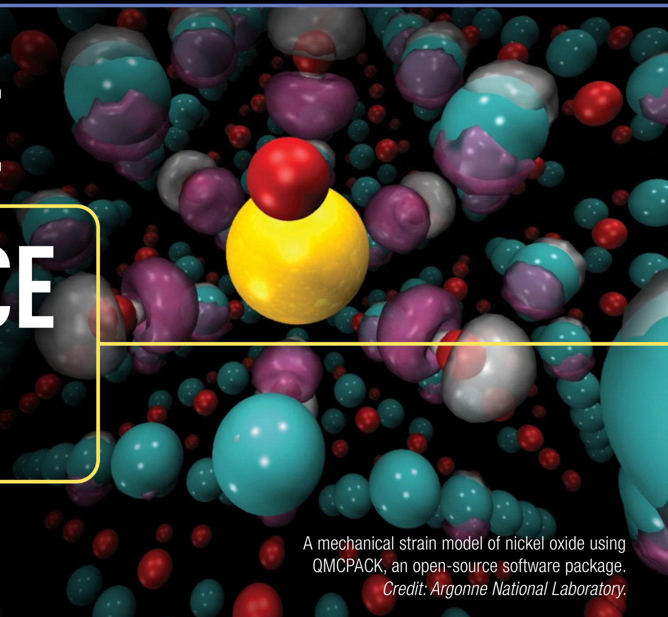
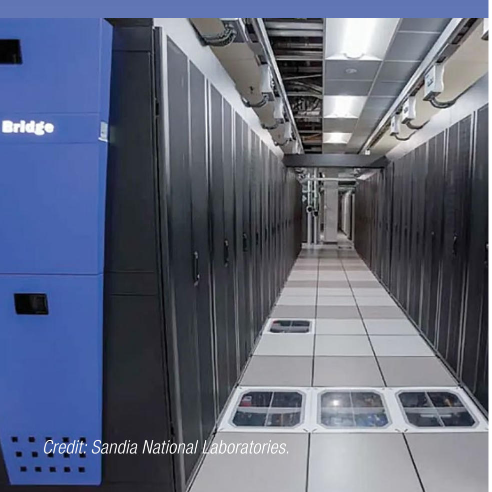
SUPPORTING SCIENCE THROUGH OPEN-SOURCE SOFTWARE

Tools Facilitate Seamless Development of New Models



A mechanical strain model of nickel oxide using QMCPACK, an open-source software package. *Credit: Argonne National Laboratory.*

Computation has accelerated the pace of scientific discovery across various fields, including engineering, materials, biology, chemistry and earth sciences. Computation complements two other approaches to scientific discovery—theory and experiment—through modeling and simulation. Simultaneously, computation relies on the complex software ecosystem that embodies scientific theory and helps researchers analyze experimental data. For decades, the Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program has provided key support of advanced scientific software through its Computer Science, Applied Mathematics and Computational Partnerships programs.



Credit: Sandia National Laboratories.

INNOVATIONS

OPEN-SOURCE SOFTWARE SPEEDS ADVANCES

Scientific software has been designed as specialized open-source components, like tools in a toolbox, freely available to the global scientific community. As a result, users can assemble complex codes quickly and use them to harness state-of-the-art high-performance computers for solving science and engineering problems. Open-source software has evolved over many decades through the pioneering contributions of ASCR researchers. A few highlights follow.

- **Since the 1970s:** The earliest mathematical software packages, EISPACK (for eigenvalue problems) and LINPACK (for solving linear equations), were developed at Argonne National Laboratory.
- **Since the 1990s:** Software components have allowed researchers to use data and computing resources efficiently on leading-edge supercomputer architectures. They also have enabled the seamless assignment of science application kernels to the processing units in flexible ways, facilitating portability on different systems.
- **Since the early 2000s:** Other software tools dovetail with scientific application codes for optimization studies, uncertainty quantification, visualization and data analysis.

IMPACT

A COMMON TOOLKIT

Virtually every discipline in science and engineering has benefited from DOE's sustained investment in software.

- Scientists don't need to become specialists in computer science and mathematics and can focus on their subject area instead.
- The ideas shared among researchers through community software have fostered new interdisciplinary collaborations across a range of institutions and accelerated scientific advancements.

TAKEAWAY

IT TAKES A COMMUNITY TO ADVANCE COMPUTING

Open-source software tools are maximizing the nation's investment in high-performance supercomputers for high-impact science and engineering.

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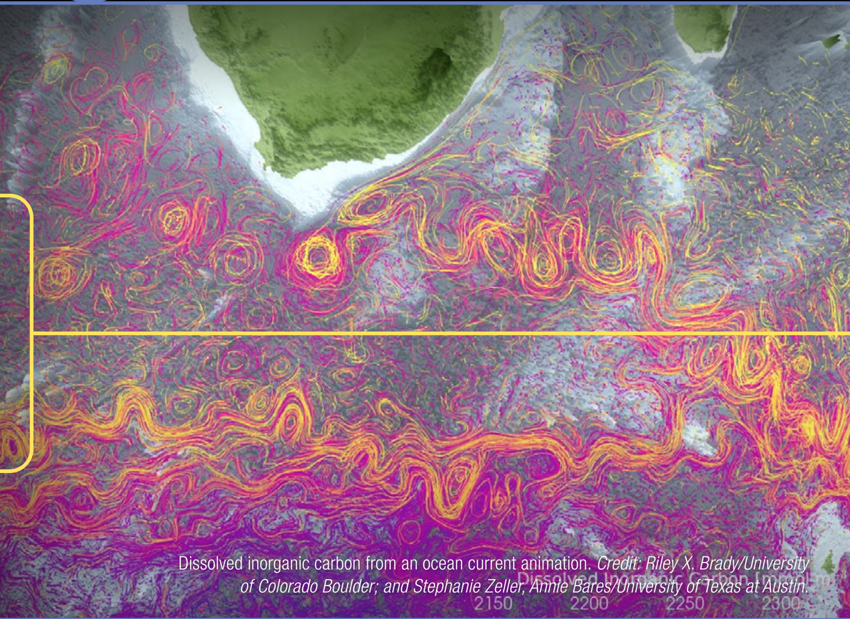
BUILDING THE COMPUTATIONAL WORKFORCE

The DOE Computational Science Graduate Fellowship



Dissolved inorganic carbon from an ocean current animation. *Credit: Riley X. Brady/University of Colorado Boulder; and Stephanie Zeller, Annie Bares/University of Texas at Austin.*

Thirty years ago, new computational scientists had to learn many skills on the job. To support and advance this evolving, interdisciplinary field, the Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program created the DOE Computational Science Graduate Fellowship (DOE CSGF) in 1991. This fellowship emphasizes multidisciplinary training and the use of high-performance computing (HPC) to develop leaders in computational science and engineering. The DOE CSGF encourages graduates to pursue national-lab careers and fosters collaborations with researchers at the labs, in academia and throughout industry.

DOE CSGF alumna Judith Hill assists fellows at an HPC workshop. *Credit: Krell Institute.*

INNOVATIONS

A NOVEL APPROACH TO TRAINING

ASCR recognized the need for interdisciplinary training in computational science early and created a unique graduate program to develop the workforce to realize this field's revolutionary potential.

- The DOE CSGF distinguishes itself from other graduate fellowships by requiring significant coursework across computation, mathematics, and science and engineering.
- Each fellow must complete a practicum at a DOE national laboratory, which provides access to advanced research, an expanded network of colleagues and mentors, the world's fastest supercomputers and forefront experimental facilities.
- DOE CSGF fellows participate in the annual program review, where they present research, learn about practicum opportunities, network with colleagues and participate in HPC training workshops.

IMPACT

A LEGACY OF LEADERSHIP

The DOE CSGF has supported more than 400 leaders in computational science and engineering who now have significant roles at the national labs, in industry and in academia.

- The vast majority (84%) of alumni remain employed as computational scientists or engineers, according to a 2017 study. Over their careers, 57% of alumni had been employed in academia, 36% in industry and 36% at a DOE laboratory.
- Alumni in academia are training the next generation of computational scientists, furthering the DOE CSGF's impact.
- Alumni serve in technical and management leadership roles within DOE and in industry; several alumni have founded technology companies.

TAKEAWAY

A WORLD-CLASS COMPUTATIONAL SCIENTIST PIPELINE

Through the DOE CSGF program, ASCR develops leaders in computational science and engineering. These efforts have placed the U.S. at HPC's forefront and have advanced HPC's role in science and engineering.

Content provided by Department of Energy multiprogram laboratory researchers. Prepared by the Krell Institute for the ASCAC Subcommittee on the 40-year History of ASCR.