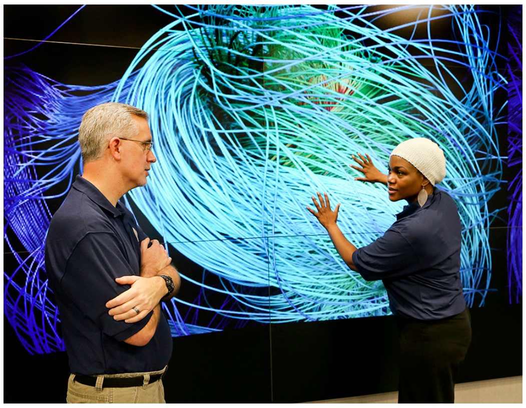
Pushing the Boundaries of High-Performance Computing

U.S. DEPARTMENT OF ENERGY

Supercomputers model and simulate complex, dynamic systems that are impractical—or impossible—to demonstrate physically. Supercomputers are changing the way scientists explore the evolution of our universe, climate change, biological systems, weather forecasting, and even renewable energy.

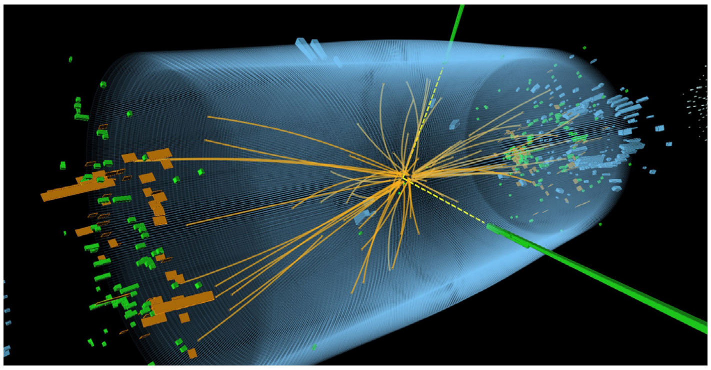
The U.S. Department of Energy's National Laboratory System has built and deployed some of the most significant high-performance computing (HPC) resources available anywhere, including 32 of the 500 fastest supercomputers in the world. Several of these computers operate at the petascale, meaning that they can perform more than one quadrillion—that's 1,000,000,000,000,000—operations per second. Though these systems rival the scale of computing power available anywhere, the National Lab System's true value lies in the scientists, engineers, and programmers who have the skills and expertise to utilize these machines to their fullest. Their ability to tackle today's most challenging computational problems while also laying the foundation for a next generation of even more powerful computers is critical not only for advancing the frontiers of human knowledge, but for helping American businesses stay at the forefront of innovation. In a fast-moving, high-tech global economy, any country that wants to remain a leading economic power will have to out-compute to out-compete.



The National Laboratory System's high-performance computing and visualization capabilities help researchers facilitate large transportation simulations using high resolution street network data at a national scale.

BIG DATA, BIG SCIENCE

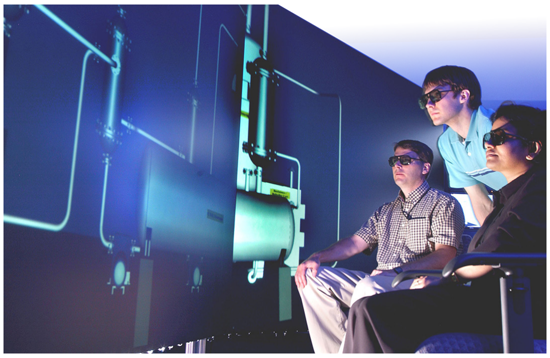
In a world of ever-increasing data, the ability to use large quantities of information to perform more accurate analyses and improve decision-making becomes even more critical. Modern supercomputers generate vast amounts of data extremely quickly as they perform detailed scientific calculations and simulations. Other scientific instruments at the National Labs, such as high-intensity x-ray light sources, also produce large quantities of data. Gathering, storing, analyzing, and interpreting data—often using different computers with various capabilities—requires unique expertise. Teamed with the National Labs' supercomputing centers and data storage facilities, and their resident Big Data experts, scientists can keep up with the volume and velocity of observations generated by today's advanced instruments to study everything from photosynthesis to the elusive and only recently discovered Higgs boson particle.



The discovery of the Higgs boson in 2012 was reported all over the world and named the Breakthrough of the Year by Science magazine. More than 1,700 U.S. scientists contributed to the Higgs boson discovery by building scientific instruments and analyzing data with the help of the DOE National Laboratory System, which contributed a large fraction of the distributed computing resources, data storage, and software infrastructure necessary to achieve this breakthrough.

THE POWER OF SIMULATION

With the computing power to handle huge numbers of operations, simulation can be used to explore many complex systems that would be impossible to observe in the laboratory. At the National Labs, simulation is being used to understand how nuclear fuel will behave inside an operating reactor, which could speed the development of safer and more efficient nuclear fuels, and to analyze the movement of chemicals through bedrock, which could help guide recovery from a chemical spill. Simulation is also helping American companies cut costs and gain a competitive edge. For example, in a recent collaboration with GE, researchers are using the National Labs' HPC resources to simulate air flow in jet engines, thereby reducing the number of wind tunnel tests needed to develop quieter and more efficient aircraft designs.



DOE's Visualization Research Group develops capabilities to visualize data and advanced power generation systems.

SOLVING PRACTICAL PROBLEMS

In addition to advancing scientific knowledge, the National Labs' deep computational resources also help solve practical problems for the American people and U.S. industry. National Lab supercomputers are being used to develop new products and improve manufacturing processes; to design high-cost, high-tech facilities, such as next-generation particle accelerators; and to deliver breakthrough energy innovations, such as the advanced materials needed to store natural gas in a solid state for new transportation applications.

The National Laboratory System's Titan computer is one of the fastest in the world, with a theoretical peak performance of more than 27 quadrillion calculations per second.

Advancing the Era of Accelerated Computing

The National Laboratory System's high-performance computers allow researchers across the scientific arena—from materials science to climate change to astrophysics—to acquire unparalleled accuracy in their simulations and achieve research breakthroughs in many critical domains more rapidly than ever before.

- **Materials Science—**High-performance computers will enable scientists to study the role of material disorder, statistics, and fluctuations in nanoscale materials and systems.
- **Combustion Dynamics—**The ability to simulate complex combustion processes will help scientists develop next-generation diesel and bio-fuels that can burn more cleanly and efficiently.
- **Climate Change—**With the computing power to combine and refine existing models for simulating global atmospheric conditions, scientists can answer questions about specific climate change adaptation and mitigation scenarios.
- **Nuclear Energy—**The ability to perform high-fidelity radiation transport calculations and reactor simulations is important in a variety of nuclear energy and technology applications.
- **Radiation Transport—**The use of supercomputers to study radiation transport has potential applications in astrophysics, laser fusion, combustion, atmospheric dynamics, and medical imaging.
- **Molecular Dynamics—**Programmers are developing multiple capability computer codes to study molecular dynamics, including membrane fusion, one of the most common ways that molecules enter and exit living cells.
- **Cosmology—**Particle astrophysicists can simulate the Big Bang and the subsequent evolution of the universe.
- **Particle Physics—**Particle accelerators, which were originally developed to investigate the fundamental laws of nature, are increasingly being used in industry. The ability to model their performance accurately using high-performance computers has major implications for U.S. competitiveness and for the development of new technologies that will impact people's daily lives.

For more information about our National Laboratory System:

DOE Website: energy.gov/science-innovation/national-labs

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