OLCF

Oak Ridge Leadership Computing Facility

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The OLCF is home to Titan, the world's most powerful supercomputer for open science with a theoretical peak performance of 27 petaflops (quadrillion calculations per second). That kind of computational capability—almost unimaginable—is on par with each of the world's 7 billion people being able to carry out approximately 3 million calculations per second. Image courtesy Oak Ridge National Laboratory

Math is the language of science, and computation, its workhorse. To accelerate answers in science and engineering, the Oak Ridge Leadership Computing Facility (OLCF), a national user facility at Oak Ridge National Laboratory, provides the open scientific community access to the world's fastest, most powerful supercomputer to address grand challenges of our time, such as improving the safety and performance of nuclear power plants and understanding climate dynamics. Titan, a Cray XK7 high-performance computing (HPC) system at the OLCF, debuted atop the list of world's fastest supercomputers in November 2012 with a calculating speed of 17.59 petaflops (quadrillion floating point operations per second). This blazingly fast supercomputer will decrease time to solution, increase complexity of models, and improve realism of simulations of subjects ranging from development of advanced materials to cleaner combustion of fuels.

In 2012, more than 1,000 researchers from industry, academia, and government used Titan's predecessor, the OLCF's 3-petaflop Jaguar—the world's fastest supercomputer from November 2009 to November 2010—to push frontiers of research and aid U.S. competitiveness in a global economy. Projects ranged from modeling hurricanes that put people and property at risk to simulating combustion instabilities that threaten the performance of power plant turbines and vehicle engines. In October of 2012, an upgrade transformed Jaguar, a machine that employed traditional central processing units (CPUs) from AMD, into Titan, a hybrid with both CPUs and graphics processing units (GPUs)—energy-efficient, high-performance chips that NVIDIA originally developed for gaming systems. Where CPUs may have up to 16 cores, GPUs have hundreds, allowing Titan to achieve 10 times the speed and 5 times the energy efficiency of Jaguar in the same physical footprint.

Titan provides a great "flops-per-watt" value for energy-efficient calculations in physics, chemistry, biology, astrophysics, engineering, and more. With the brawn of GPUs to exploit massive parallelism in scientific application codes, Titan's hero-scale simulations will explore topics from the exotic behavior of magnetic nanomaterials to the commercially viable production of cellulosic ethanol. With Jaguar, scientists could simulate combustion of simple fuels used as laboratory reference standards. With speedier Titan, they will be able to simulate the complex fuel blends we put in our gas tanks. Moreover, Titan will empower scientists to ask new types of questions. With Jaguar, seismologists wanting to assess regional risks could ask how a single earthquake might propagate in three dimensions. With game-changing Titan, however, they will be able to pinpoint hundreds of earthquakes worldwide and work backward using "inverse tomography" to ask what forces cause all those quakes.

Unmatched resources and expertise

The first major computing system to employ a hybrid architecture, Titan features 18,688 compute nodes, a total system memory of 710 terabytes, and Cray's high-performance Gemini network. Its 299,008 CPU cores guide simulations while accompanying GPUs do the heavy lifting. OLCF resources for data analysis and visualization include the Lens and Smoky clusters and the Exploratory Visualization Environment for REsearch in Science and Technology, or EVEREST. File systems such as Spider for immediate data storage, with more than 240 gigabytes per second of aggregate throughput and more than 10 petabytes of storage capacity, and the High Performance Storage System for archival data storage, manage the floods of data that Titan's simulations generate. All of these resources are available through high-performance networks including ESnet's recently upgraded 100 gigabit per second links.

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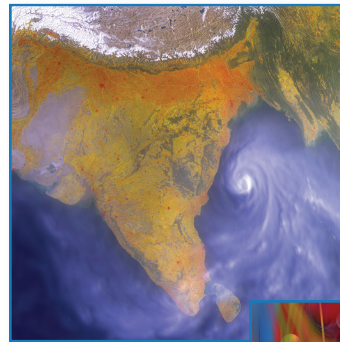
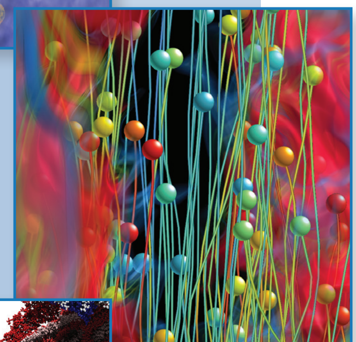
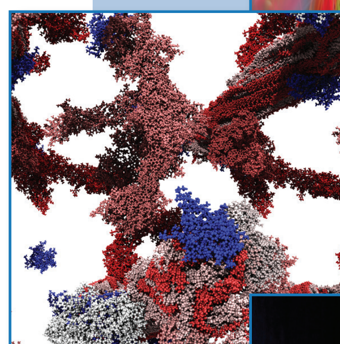
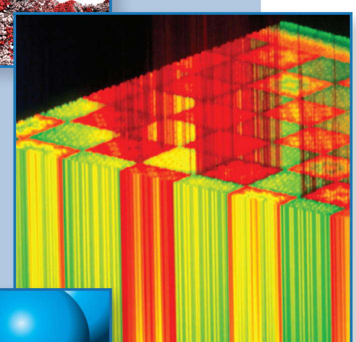
To help Titan's users make the most of premier high-performance supercomputing, data storage, and scientific visualization facilities, OLCF experts engage deeply with users to develop and scale scientific application codes to run on the world's most powerful supercomputer. They provide users access to HPC systems and training to make the most of the resources. They develop software tools to improve the performance of applications on extreme-scale systems; install, test, and operate hardware; ensure cybersecurity; and update and integrate technologies. OLCF's Ph.D.-level computational scientists collaborate with users to maximize science output for the projects. Experts in code development, data analysis, and visualization support users, turning the numeric data into scientific insight.

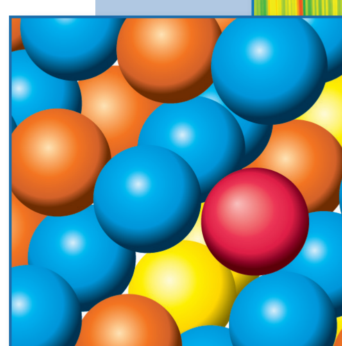
The OLCF's cutting-edge facilities and support systems are available through three programs that allocate millions of processor hours to top-tier computational scientists. The Innovative and Novel Computational Impact on Theory and Experiment program supports large-scale, high-impact projects that make concurrent use of at least 20 percent of Titan's cores. The Advanced Scientific Computing Research Leadership Computing Challenge, or ALCC program, primarily aids research that supports the energy mission of the Department of Energy's Office of Science, such as advancing clean energy and understanding environmental consequences of energy use, and emphasizes high-risk, high-rewards endeavors. And the OLCF's Director's Discretionary program helps new HPC users explore topics of national importance.











Research achievements

Titan's sponsor, the DOE Office of Science, is the single largest supporter of basic research in the physical sciences in the United States and is working to address some of the most pressing challenges of our time. To better understand the natural world and to spur improvements in the engineered world, OLCF supercomputers have simulated supernovas in 3D, modeled tomorrow's turbomachines, optimized clean combustion for power and propulsion, and helped pinpoint the molecular basis of Parkinson's disease. The have enabled major insights in climate science, nuclear physics, chemistry, materials science, and more.

Making the most of supercomputers largely means exploiting parallelism to deliver more science. Titan's predecessor, Jaguar's, amply demonstrated its impact on scientific supercomputing with several Gordon Bell prizes, which recognize outstanding HPC applications and assess progress in parallel computing. Researchers expect Titan to set the bar even higher by delivering petascale science results from day one in diverse fields. In materials science, illuminating the world at the atomic and molecular level will unravel secrets of superconductivity, catalysis, and electronics. Simulations of Earth's complex climate system will allow researchers to explore areas including abrupt climate change, the influence of clouds, and century-long ocean circulation patterns. And in fusion energy, the process that drives the stars may one day provide us with clean, limitless electricity. But scientists must first understand how to control a plasma that is hotter than the sun by simulating magnetic fields that constrain the fuel, radio waves that heat it, and turbulence that complicates the process. These are but a few of the daunting problems that science and engineering can address. Titan stands at the ready to speed solutions.

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