

OAK RIDGE LEADERSHIP COMPUTING FACILITY

POWER TO THE PEOPLE

How the Jaguar supercomputer helps assure America's energy security



“So we have a choice to make.

We can remain one of the world’s leading importers of foreign oil, or we can make the investments that would allow us to become the world’s leading exporter of renewable energy. We can let climate change continue to go unchecked, or we can help stop it. We can let the jobs of tomorrow be created abroad, or we can create those jobs right here in America and lay the foundation for lasting prosperity.”

—President Obama, March 19, 2009

Supercomputing can inform our choices about energy. We need a diverse portfolio of solutions to meet growing energy demands sustainably, and that means innovative research and development. The Department of Energy (DOE) provides unparalleled high-performance computing resources for the scientific community. Today’s grand challenges in science and engineering are too complex for soloists to solve. Simulations help research teams explore complex, dynamic scenarios.



Four of the world’s 25 swiftest supercomputers are at the Oak Ridge Leadership Computing Facility (OLCF) on the Oak Ridge National Laboratory (ORNL) campus. The fastest is a powerful Cray XT system called Jaguar with a theoretical peak calculating speed of more than 2 petaflops, or quadrillion calculations per second. With almost a quarter of a million AMD Opteron processing cores working together, Jaguar can do in a day what it would take every person on Earth several hundred years to do—assuming each could complete one calculation per second. Its unparalleled memory, analysis and visualization clusters, input/output bandwidth, and scalable storage system are ideal for manipulating, analyzing, moving, and storing massive data from simulations.

Researchers from industry, academia, and government depend on supercomputers at the ORNL computing complex to tackle compelling challenges. Through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, jointly managed by Leadership Computing Facilities at Oak Ridge and Argonne national laboratories, researchers in 2009 were allocated about 470 million hours on Jaguar. In 2010 researchers will receive 1 billion processor hours on Jaguar.

From energy conservation to carbon capture and storage, supercomputers explore “What if?” scenarios. If batteries are reengineered, can they store enough charge to increase the range of electric vehicles? If the world’s farmers plant more biofuel crops, how will that affect global climate? If utilities deploy “smart” electrical grids, how much energy can consumers save? Supercomputing speeds answers. Below are the goals of some DOE supercomputing projects to assure our energy supply.

Boost gas mileage. Fuel efficiency could improve by at least 25 percent if next-generation vehicles burn lean fuel mixtures in low-temperature, compression-ignition engines. In simulations of burning fuel led by Jacqueline Chen of Sandia National Laboratories, Jaguar generated 120 terabytes (trillion bytes) of data about ignition and stabilization of flames. That’s more than five times the printed contents of the U.S. Library of Congress. Engineers use this combustion data to aid design of vehicle engines and industrial boilers with reduced emissions and increased efficiency.

Make materials for energy efficiency. Aided by simulations, materials scientists are inventing high-temperature superconductors to transmit energy with little resistance and improved magnets to drive motors in electric vehicles. Engineering stronger steels with fewer misaligned iron atoms, they may be able to reduce the amount of metal needed in vehicles. The lighter-weight vehicles will require less energy to move. The researchers also investigate the storage and

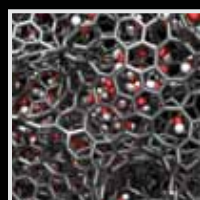
flow of energy in novel electrochemical devices that surpass the performance of conventional batteries. Moreover, they characterize the atomic properties of materials that absorb light and transmit electrons to find ways to improve the efficiency of solar panel materials.

Squeeze more energy out of biomass. Cellulose, a complex carbohydrate that forms the cell walls of plants, gives leaves, stalks, stems, and trunks their rigidity. Figuring out how to unlock its sugar subunits, which can be fermented to produce ethanol, could enable full use of plants for fuel. At the ORNL computing complex, Jeremy Smith leads a team of researchers from the University of Tennessee and ORNL in simulating cellulose in unprecedented detail to reveal its structure, motion, and mechanics. The new knowledge may spawn cell walls that are less resistant to decomposition and enzymes that are more efficient at breaking down cellulose.

Burn coal more cleanly. Researchers use Jaguar to speed and optimize the design of advanced power plants to tap coal’s oxidative potential and trap its pollutants. Near-zero-emission facilities would burn gasified coal to generate electricity and hydrogen and sequester carbon dioxide. Instead of building an expensive prototype plant and seeing how effectively it burns coal, engineers can model a prototype, simulate its performance, and adjust operating conditions in hundreds of virtual experiments to learn what works best before they build.

Reduce nuclear waste. One way to reduce nuclear waste is to fuel a fast reactor with it. But the enormous expense of experiments has slowed development of a commercially viable fast reactor. Simulating the behavior of neutrons and other particles in reactors, Jaguar performs lightning-fast calculations involving billions of spatial elements, thousands of energy groups, and hundreds of angles. The improved fast reactor designs that result could greatly reduce the volume of waste from nuclear power plants.

Develop fusion for the future. Simulations help researchers understand how to make the most of radio waves to heat and control plasma, the ionized gas that fuels fusion reactors. They support ITER, an endeavor toward developing commercial fusion power plants. Antennas will launch radio waves carrying 20 megawatts—the power equivalent of a million compact fluorescent light bulbs—into the reactor. The waves will heat deuterium and tritium fuel to form plasma and drive currents to confine the plasma. Success means harnessing the process that powers the sun to provide clean, abundant energy here on Earth.



Petascale Jaguar:

Balancing speed and power to solve complex problems