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INCITE grants awarded to 59 computational research projects

Nov. 18, 2013--The U.S. Department of Energy's Office of Science announced 59 projects, promising to accelerate scientific discovery and innovation, that will share nearly 6 billion core hours on two of America's fastest supercomputers dedicated to open science. Their work will advance knowledge in critical areas from sustainable energy technologies to the environmental consequences of energy use.

The allocations come from the Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, program. Through it, the world's most advanced computational research projects from academia, government, and industry are given access to the Department of Energy's (DOE's) leadership computing facilities at Oak Ridge and Argonne national laboratories.

"The INCITE program addresses the largest, most computationally pressing projects in science and engineering," said Michael Papka, director of the Argonne Leadership Computing Facility (ALCF). "These allocations enable state-of-the-art science in a wide range of domains."

"The INCITE program—which is celebrating its 10-year anniversary—provides researchers with the opportunity to make scientific breakthroughs in fields that would not be probable or even possible without access to the most powerful available supercomputers," said James Hack, director of the National Center for Computational Sciences, which houses the Oak Ridge Leadership Computing Facility (OLCF).

When INCITE made its first awards in 2004, three projects received an aggregate five million hours on DOE supercomputers. Today's collective allocation of nearly 6 billion core hours represents a 1,000-fold growth in resources provided to researchers. The average award is more than 75 million core hours—with individual awards of up to several hundred million core hours—on systems capable of quadrillions of calculations each second.

The ALCF's primary leadership computing resource is Mira, a 10-petaflops IBM Blue Gene/Q system with 49,152 compute nodes and a power-efficient architecture. The OLCF's Titan supercomputer is a 27-petaflops Cray XK7 hybrid system employing both CPUs and energy-efficient, high-performance GPUs in its 18,688 compute nodes.

Despite continued upgrades and expansions, demand for leadership computing facilities surpasses availability, and DOE's world-class facilities continue to attract new users. This year INCITE applications greatly exceeded awards.

“INCITE is one of the main programs that gives researchers access to some of the country’s leadership computing facilities,” said Julia White, INCITE manager at DOE’s Leadership Computing Facilities. “Large supercomputer awards like this also give researchers support from computer experts who design code and optimize it for the supercomputers, which helps ensure that the scientists who run simulations on DOE’s machines can take full advantage of their enormous processing power.”

Supercomputer simulations create a detailed picture of complex phenomena by relying on codes packed with math equations. For a complete list of 2014 INCITE awards, see <http://www.doeleadershipcomputing.org/awards/2014INCITEFactSheets.pdf>. Highlights of the 2014 allocations include the following:

- Michael Klein of Temple University and a research team from Procter & Gamble received 75 million core hours to simulate the cohesive forces between the microscopic layers of human skin and evaluate the impact of chemicals on skin.
- Anne Laure Dord from GE was awarded 75 million core hours to guide the design of future aircraft engines.
- Larry Curtiss from Argonne and a research team from IBM received 100 million core hours to address the chemical and physical mechanisms that could lead to breakthroughs for lithium air batteries.
- Thomas Jordan from the University of Southern California leads a project that was awarded 112.2 million core hours to uncover the physics of earthquake processes, potential seismic hazards from known earthquake faults, and impact of strong ground motions on modern buildings.
- Poul Jørgensen from Aarhus University in Denmark received 24 million core hours to study supramolecular wires that are made of a new class of organic gel.
- James Amundson from Fermilab was awarded 50 million core hours to simulate Fermilab and CERN accelerators that could enable future discoveries in the Intensity and Energy Frontiers of particle physics.

DOE’s 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.

The INCITE program promotes transformational advances in science and technology through large allocations of time on state-of-the-art supercomputers. For more information, see <http://www.doeleadershipcomputing.org/incite-program/>.

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