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Supercomputing Award of 5.95 Billion Hours to 55 Computational Research Projects

Oak Ridge, Tenn., Nov. 13, 2017—The U.S. Department of Energy's Office of Science announced 55 projects with high potential for accelerating discovery through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The projects will share 5.95 billion core-hours on three of America's most powerful supercomputers dedicated to open science and support a broad range of large-scale research campaigns from infectious disease treatment to next-generation materials development.

These awards allocate the multi-petascale computing resources of two DOE Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories. The two centers jointly manage the INCITE program as is the primary means of accessing their resources. INCITE proposals are awarded on a competitive basis to researchers from academia, government research facilities, and industry. The average award is more than 108.1 million core-hours—with some awards of up to several hundred million core-hours—on systems capable of quadrillions of calculations per second.

"DOE's INCITE program gives researchers access to computational resources to ambitiously address some of the world's most formidable scientific research problems," said James Hack, director of the National Center for Computational Sciences (NCCS), home to the Oak Ridge Leadership Computing Facility (OLCF), a DOE Office of Science User Facility in Oak Ridge, Tennessee. "These scientific projects would not be possible without access to DOE leadership computing resources, and we're gratified to be able to partner with these outstanding research teams to enable fundamental advances in our understanding of the amazing world in which we live."

Domain scientists and computational scientists at the leadership centers partner with each INCITE project, aiding in code and methods development, optimization, streamlining workflow, troubleshooting unforeseen problems, and assisting with data analysis and visualization.

"Researchers seek out the INCITE program to support their research through access to three of the world's fastest supercomputers, but our facilities also provide significant staff expertise and support to help them achieve their goals," said Michael E. Papka, director of the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science User Facility just outside Chicago. "This support helps ensure investigators can maximize their time on our leading-edge systems."

The ALCF's Mira supercomputer is a 10-petaflops IBM Blue Gene/Q system with 49,152 compute nodes and a power-efficient architecture. ALCF's Theta is a 9.65-petaflops Cray XC40

system based on the second-generation Intel Xeon Phi processor. 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, expansions, and advances in computing power, demand for leadership-class resources such as Mira, Theta and Titan continues to exceed availability, and, once again, more applications for time were made to INCITE than were awarded.

For a complete list of 2018 INCITE awards, please visit:
http://www.doeleadershipcomputing.org/awards/2018INCITEFactSheets.pdf

Highlights of the 2018 allocations include:

- Brant Robertson from the University of California Santa Cruz received 46 million core-hours to understand the role galactic-scale winds play in the formation and evolution of galaxies.
- Rommie Amaro from the University of California San Diego received 80 million core-hours to investigate the druggability and transmissibility of pandemic and seasonal influenza. These simulations, the largest of their kind, will unlock new clues to flu infection and potential treatment.
- Michael Sprague from DOE's National Renewal Energy Laboratory received 115 million core-hours to create new predictive simulation capabilities that will lower the cost of wind energy by providing new understanding and new pathways to optimized wind farms.
- Vasily Bulatov from DOE's Lawrence Livermore National Laboratory received 110 million core-hours for large-scale molecular dynamics simulations that will increase understanding of the strength of construction materials by understanding both the microscopic origin of strain hardening and the nature and geometric character of dislocation patterns.
- Sean Dettrick from TAE Technologies received 31 million core-hours for simulations in understanding the magnetic confinement of plasmas with the goal of creating a clean, commercially viable, fusion-based electricity generator.
- Konstantinos Orginos from the College of William & Mary received 155 million core-hours to study the structure of hadrons that will allow, for the first time, a complete 3D image of the hadron using the fundamental theory known as Quantum Chromodynamics.

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

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. For more information, please visit http://science.energy.gov.