Supercomputers Take Science By Storm

EurekAlert

Five researchers at the U.S. Department of Energy's (DOE) Argonne National Laboratory will lead projects that have been awarded almost 200 million processor-hours of computing time at Argonne's Leadership Computing Facility (ALCF). The ALCF is home to an IBM Blue Gene/P, a supercomputer capable of performing 557 trillion calculations per second, enabling scientists and engineers to conduct cutting-edge research in weeks or months rather than years.

"By providing millions of hours of computing time on this powerful system, these awards allow us to address some of the nation's most challenging scientific problems," said Pete Beckman, director of ALCF.

Chosen through a peer review process, the following Argonne projects have been selected by DOE to run at the ALCF as part of the new ASCR Leadership Computing Challenge (ALCC).

- Andrew Siegel, a computational scientist and leader of Argonne's nuclear simulation activities, was awarded 75 million hours to investigate vibrations caused by turbulent flow in the core of light-water reactors. Simulating these behaviors will help optimize reactor fuel use, as well as advance our understanding of computational fluid dynamics.

- Micheal Smith, an Argonne nuclear engineer, was awarded 38 million hours for the analysis and design of sodium-cooled fast reactors. This research is crucial in the development of nuclear reactors that are safe, affordable and environmentally friendly. It also represents one of the most challenging multiphysics simulation problems, which requires coupling neutronics simulation together with thermo-fluid and structural analysis simulations.

- Michael Borland of Argonne's Advanced Photon Source (APS) was awarded 36 million hours to optimize the configuration of magnets as part of a planned upgrade to the APS - a world-class source of high-energy, tunable X-rays for scientific research. Borland will use an innovative genetic optimization technique to rapidly design changes in magnet configuration needed for the upgrade that do not impact existing operating modes of the APS.

- Benoit Roux, a senior computational biologist at Argonne and senior fellow of the Computation Institute, was awarded over 28 million hours to develop new computational approaches for studying complex biological

macromolecular systems. His research will entail cutting-edge modeling to simulate the activation of membrane-associated proteins that function as molecular switches, advancing our understanding of the structure, dynamics and function of biological systems.

- Larry Curtiss of Argonne's Center for Nanoscale Materials was awarded 20 million hours for the design and discovery of new materials critical to our energy future. His team will focus on electrical energy storage and catalytic materials leading to safer, more energy-efficient and environmentally friendly battery technologies for long-range electric vehicles and efficient conversion of biomass to light fuels.

Other projects awarded by the ALCC to run at Argonne's ALCF include the following:

- Researchers from the National Oceanic and Atmospheric Administration (NOAA) will run ultra-high-resolution global climate simulations tracking selected hurricanes.

- Scientists from GE will simulate advanced aircraft propulsion technologies, to improve fuel efficiency and reduce noise.

- Stanford University scientists will collaborate with Argonne scientists to enable very-large-scale turbulence simulations.

- Researchers from MIT will perform an unprecedentedly realistic calculation of nucleon structure using full lattice quantum chromodynamics.

Open to researchers from national laboratories, academia and industry, the ALCC program allocates up to 30 percent of DOE's computational resources at the National Energy Research Scientific Computing Center (NERSC) and the Leadership Computing Facilities at Argonne and Oak Ridge. The program focuses on high-risk, high-payoff simulations in mission-critical areas such as advancing clean energy and understanding the Earth's climate. More information about ALCC is available online.

The ALCF is dedicated to large-scale computation and builds on Argonne's strengths in high-performance computing software, advanced hardware architectures and applications expertise. The ALCF's Blue Gene/P, named "Intrepid," is one of the fastest and most energy-efficient supercomputers in the world. It features more than 160,000 processors and over 80 terabytes of memory. ALCF staff also provide

the computational expertise and support to help scientists optimize and scale their applications to maximize the use of these powerful resources.

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