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OLCF Selects Application Readiness Projects to Prepare for Next-Generation Summit Supercomputer

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Newswise — OAK RIDGE, Tenn., April 15, 2015—The U.S. Department of Energy's (DOE) Oak Ridge Leadership Computing Facility (OLCF) has selected the next set of partnership projects into its Center for Accelerated Application Readiness (CAAR) program. The program brings together application development teams and staff from the OLCF Scientific Computing group to prepare for Summit, the OLCF's next leadership-class computing system for open science.

Summit, a high-performance computing system set to be delivered to Oak Ridge National Laboratory (ORNL) in 2017 and available to researchers in 2018, will support DOE's Office of Science in its broad science and energy mission, advancing knowledge in areas critical to government, academia and industry.

The CAAR program is focused on optimizing application codes for Summit's hybrid architecture, which includes IBM POWER CPUs, NVIDIA® GPU accelerators and the NVLink™ high-speed interconnect technology. Summit is expected to provide at least five times the performance of the OLCF's current leadership system, Titan. Leading up to the delivery of Summit, the CAAR application teams, with technical support from the IBM/NVIDIA Center of Excellence at ORNL, will redesign, port and optimize their software to Summit's architecture and demonstrate the

effectiveness of their application on Summit through a scientific grand-challenge project.

"We know that improved software is just as important as improved hardware to supercomputer performance and our facility's mission," says Dr. Tjerk Straatsma, ORNL's Scientific Computing group leader. "CAAR brings together the people who know the science, the people who know the code, and the people who know the machine so that cutting-edge science can be conducted on Summit."

In addition to resources at the OLCF, including Titan and early software development systems for Summit, the CAAR teams will have access to computational resources at the Argonne Leadership Computing Facility (ALCF) and the National Energy Research Supercomputing Center (NERSC) at Berkeley Lab to enable architecture and performance portability across different computing architectures.

These projects were chosen based on a computational and scientific review conducted by the OLCF in consultation with the ALCF, NERSC, IBM and NVIDIA. The application teams represent a broad range of computational algorithms and programming approaches in a diverse range of scientific disciplines including astrophysics, biophysics, chemistry, climate modeling, combustion engineering, materials science, nuclear physics, plasma physics and seismology.

"We had a tremendous response to our call for proposals, receiving a large number of strong entries," Straatsma said. "The diversity of the selected applications gives us the opportunity to develop highly scalable, highly efficient applications for Summit that many of our users can take advantage of when the machine comes into production."

The modeling and simulation applications selected for the CAAR program and their principal investigators include:

Climate simulation code ACME, Dr. David Bader, Lawrence Livermore National Laboratory
Relativistic chemistry code DIRAC, Prof. Lucas Visscher, Free University of Amsterdam
Astrophysics simulation code FLASH, Dr. Bronson Messer, Oak Ridge National Laboratory
Plasma physics code GTC, Dr. Zhihong Lin, University of California-Irvine
Cosmology simulation code HACC, Dr. Salman Habib, Argonne National Laboratory
Electronic structure application LS-DALTON, Prof. Poul Jørgenson, Aarhus University
Biophysics simulation code NAMD, Prof. Klaus Schulten, University of Illinois at Urbana-Champaign

Nuclear physics application NUCCOR, Dr. Gaute Hagen, Oak Ridge National Laboratory
Computational chemistry code NWCHEM, Dr. Karol Kowalski, Pacific Northwest National Laboratory

Materials science application QMCPACK, Dr. Paul Kent, Oak Ridge National Laboratory
Combustion engineering code RAPTOR, Dr. Joseph Oefelein, Sandia National Laboratories
Seismology application SPECFEM, Prof. Jeroen Tromp, Princeton University
Plasma physics code XGC, Dr. C.S. Chang, Princeton Plasma Physics Laboratory

For more information on the CAAR program, visit www.olcf.ornl.gov/caar.

The OLCF is a DOE Office of Science User Facility established at ORNL in 2004 with the mission of accelerating scientific discovery and engineering progress by providing outstanding computing and data management resources to high-priority research and development projects. Along the way it has delivered two-world leading systems. The first supercomputer, a Cray XT known as Jaguar, ran the first scientific applications to exceed 1,000 trillion calculations per second (1 petaflop) and ranked as the world's fastest computer in November 2009 and June 2010 on the Top500 list. The OLCF continued to expand the limits of computing power, unveiling Titan in 2013, a hybrid Cray XK7 capable of 27 petaflops. Titan was recognized as the world's fastest in November 2012.

For more information about Summit, visit: https://www.olcf.ornl.gov/summit.

UT-Battelle manages ORNL for the DOE's Office of Science. The Office of Science is the single largest supporter

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Image: http://www.ornl.gov/Image%20Library/Main%20Nav/ORNL/News/News%20Releases/2015/Summit-2.jpeg

Caption: The Oak Ridge Leadership Computing Facility is preparing for Summit, the OLCF's next leadership-class computing system, through its Center for Accelerated Application Readiness program.

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