Theta Takes on Astronomy, Cosmology and Neuroscience

CASE STUDY : : ALCF

ARGONNE LEADERSHIP COMPUTING FACILITY

MULTI-DISCIPLINARY

ACCELERATING SCIENCE

THE THETA EARLY SCIENCE SUPERCOMPUTING SYSTEM IS PAVING THE WAY FOR A NEW GENERATION OF ULTRA-HIGH PERFORMANCE SUPERCOMPUTERS.

SOLUTION CHOICE

Cray® XC™ series supercomputer

Cray® Sonexion® storage system

SYSTEM DETAILS

Peak performance: 8.5 PF

Nodes: 3,240

File System Capacity: 10 PB

File System Throughput: 210 GB/s

CRAY XC BENEFITS

- Supports different processing and storage technologies
- Integrated software ecosystem
- Optimizes applications for best performance and memory usage

CRAY SONEXION BENEFITS

- Scales performance and capacity more efficiently than conventional Lustre solutions
- Up to 38% more throughput per rack
- Reduces TCO by up to 25%
- Pre-integrated and fully tested with single point of support

BACKGROUND: MOVING TOWARD EXASCALE — The Department of Energy's CORAL program is a $525 million initiative to build state-of-the-art supercomputers five to seven times more powerful than today's top systems.

CORAL, or the joint collaboration of Oak Ridge, Argonne and Lawrence Livermore national laboratories, will culminate in three ultra-high performance supercomputers. A first-of-its-kind effort, the resulting systems will be used for the most demanding scientific and national security simulations and modeling — and move the industry another step closer to exascale-level computing.

For its part, "Theta" is the first of two systems at the Argonne Leadership Computing Facility (ALCF). An early production system, Theta is paving the way for "Aurora," a next-generation Cray supercomputer and high-performance storage system due for delivery in 2018 and designed to deliver 180 PF of peak compute performance.

Theta is based on the Cray® XC™ series supercomputer with second-generation Intel® Xeon Phi™ "Knights Landing" processors. It boasts 8.5 PF of peak compute performance and 10 PB of storage provided by the Cray® Sonexion® scale-out Lustre® system.

As part of the effort to prepare scientific applications for the architecture and scale of the Theta, and subsequent Aurora systems, ALCF launched the Theta Early Science Program (ESP). The program brings together computational scientists, code developers and computing hardware experts to optimize key applications and solidify libraries and infrastructure.

This case study highlights two of those research projects and how the teams plan to use Theta's capabilities.

CRAY

THE THETA EARLY SCIENCE PROGRAM SUPPORTS INNOVATIVE SCIENCE NOT POSSIBLE ON TODAY'S LEADERSHIP-CLASS SYSTEMS.

USE CASE: Next-Generation Cosmology Simulations

As the next generation of cosmological surveys starts taking data, a major challenge will be separating astrophysical effects from fundamental physics.

This early science project aims to understand the impact of baryons by coupling hydrodynamics into gravitational simulations of the mass evolution of the universe. Through this work, the ESP team will build new capabilities for the extreme-scale Hardware/Hybrid Accelerated Cosmology Code (HACC) and advance understanding of astrophysical processes.

To achieve their goals, the research team has to understand the physics of the universe on ever-smaller scales. Access to Theta is critical to the undertaking.

Specifically, the team will carry out a suite of large-volume simulations — some of the largest hydrodynamics simulations thus far. One particular simulation is of such high-mass resolution that it will require the entire Theta system.

The team expects to benefit from the node-local solid-state disks which will be large enough to hold a single checkpoint file for HACC. Additionally, the Cray Aries™ interconnect will enable scaling the long-range force calculation efficiently to large numbers of Theta nodes.

Additionally, the system size will enable a number of code optimization tasks. Chief among them is optimizing the short-range solver for the Intel Xeon Phi processor. Theta offers them a first-ever opportunity to do so.

USE CASE: Large-Scale Simulation of Brain Tissue

The brain remains the body's least-understood organ. Integration through data-driven brain tissue models offers a novel method for gaining insight. In service of that effort, the Blue Brain Project (BBP) formed in 2005 to enable the integration of heterogeneous neuroscience data into unifying models for simulation-based research.

Working with neuroscientists, the project has designed a software infrastructure resulting in a first-ever opportunity to perform "in silico" experiments on virtual tissue — something impossible experimentally thus far. But detailed brain tissue models represent a computational grand challenge, so this ESP project will use the Theta system to explore and assess the suitability of next-generation supercomputers for these problems. Overall, the project will advance simulation tools, widen scientific questions on brain plasticity and prompt discussions within the HPC community.

Specifically, the team aims to test various aspects of system memory through several scientific applications: simulations of neocortical columns, simulations of the electrical activity of the somatosensory cortex, and a simulation of the electrical activity of the largest-possible brain model for several seconds.

ABOUT ALCF

The Argonne Leadership Computing Facility accelerates major scientific discoveries and engineering breakthroughs for humanity by designing and providing world-leading computing facilities in partnership with the computational science community.

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Cray provides systems and solutions that help you solve your most difficult computing, storage and data analytics challenges. Our portfolio includes powerful supercomputers, optimized cluster systems, advanced storage systems and data analytics and discovery platforms.

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