Celebrating Science at the Petascale

Scientific discovery has entered the age of petascale computing with the Department of Energy's Office of Science leading the way, with both the systems and the scientists to tackle the nation's most important challenges.

These challenges are pressing and immediate, led, not surprisingly, by questions of climate change and energy assurance. Climate and energy studies are among the most high-profile research areas supported through the Office of Advanced Scientific Computing Research's INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program, and our efforts in these areas promise the most direct benefit to society.

Scientists will continue to increase the fidelity by which we are able to explore the Earth's climate system. With supercomputers that have been installed—or will soon be installed—we expect to realistically evaluate our ability to predict climate change at the regional level and give resource managers the tools they need to plan effectively for the future. We will also apply these new computing systems to help guarantee that the country's energy needs are met with as little economic or environmental disruption as possible. We look forward to new insights into the atomic and molecular building blocks of biomass, insights that will lead the way to mass production of cellulosic bioethanol. We also expect to see continuing improvements in our understanding of combustion, which in turn will help us squeeze as much energy as possible from existing fossil fuels, and of new generations of nuclear energy, both fusion and fission. We further anticipate new and improved energy storage technologies to emerge as a result of these tremendous scientific tools now at our disposal.

It is impossible in one column to do justice to the range of important science being conducted at our computing centers, but we expect profound new discoveries on scales ranging from the behavior of subatomic particles to the future of the Universe.

We are confident in our ability to deliver on these efforts, as evidenced by the SC08 conference recently held in Austin, Texas. This annual gathering of computer experts and computational researchers gives us many of the measures we use to evaluate our performance as a community. Time and again, Office of Science systems and researchers were at the top of the list.

The best-known measure of HPC systems is found in the Top500 List, which compares the raw speed of leading supercomputers with the High-Performance Linpack test. By this measure alone, we could say that the Office of Science operates four of the world's eight most powerful supercomputers, or five of its top 20 systems. Oak Ridge National Laboratory's (ORNL) Cray XT5 Jaguar system demonstrated beyond doubt that the Office of Science has entered the petascale age by achieving a sustained 1.059 quadrillion mathematical calculations a second, or 1.059 petaflops. This system also possesses an impressive 300 TB of memory, which is three times more any other current supercomputer.

An even more valuable test of these systems' value comes from a series of tests known together as the HPC Challenge, which probe a system's ability to execute the types of operations and algorithms imperative for scientific discovery. Office of Science systems showed that they are the best in the world by coming out on top of all four of the tests included in this challenge. Argonne National Laboratory's Blue Gene/P Intrepid system showed the strongest performance in the Global Random Access competition, which measures random memory access performance, and in the Global Fast Fourier Transformation, a common algorithm used in many scientific applications. ORNL demonstrated the power of its Cray XT Jaguar system by coming out on top of the test for solving a dense matrix of linear algebra equations and sustainable memory bandwidth, which measure how many gigabytes per second a node can fetch and store.

ORNL

Dr. Thomas Zacharia with "Jaguar," ORNL's powerful Cray XT.

More important than the systems, of course, are the applications running on them. There, too, the Office of Science was in the spotlight. Each year, the Gordon Bell Prize recognizes the world's most advanced scientific computing applications. In 2008, there were two prizes, both going to researchers at Office of Science laboratories running their applications on Office of Science systems. The performance category award went to a team led by ORNL's Thomas Schulthess (recently named director of the Swiss National Supercomputing Center at Manno), which achieved a sustained performance of 1.352 petaflops on Jaguar for an application that delves into the behavior of high-temperature superconductors. A second award, this one in the special category for innovation in algorithms, went to a team led by Lin-Wang Wang of Lawrence Berkeley National Laboratory (LBNL) for an application that allows researchers to tackle electronic systems of thousands to tens of thousands of atoms that can be simulated accurately only by *ab initio* methods. Wang's team ran its application on three separate Office of Science supercomputers, including LBNL's Cray XT4 Franklin system, as well as Jaguar and Intrepid.

Given these resources, the Office of Science is able to continue offering unprecedented levels of computing resources to the world's most talented computational researchers. It should not be surprising that we are optimistic about the future.

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