National Center for Computational Sciences Snapshot
The Week of April 16, 2007

Meeting Charts a Path to the Future

NCCS users and staff look to petascale and beyond

More than 70 National Center for Computational Sciences (NCCS) users and others interested in the center recently gathered at Oak Ridge National Laboratory (ORNL) to discuss the center's direction, network with staff and one another, and hone their skills.

The second annual NCCS Users Meeting—held March 27–29—also allowed researchers to discuss the work they are performing on the center's state-of-the-art systems and outline their needs as the NCCS moves to petascale systems and beyond.

High-performance computing (HPC) has become a national priority, explained Barbara Helland, program manager for the Department of Energy's Office of Advanced Scientific Computing Research. Helland pointed to President Bush's 2006 State of the Union address, which called for increased funding for research throughout the physical sciences, including supercomputing. She stressed, however, that advances in computing are only a means to an end.

"Even though we've put the facilities here," she told users "you're the important piece in the puzzle because you're going to use these facilities for scientific discovery and breakthrough. We're not in it to build the facility and have the fastest machine; we're in it for scientific accomplishment."

ORNL Leadership Computing Facility (LCF) Director Buddy Bland noted that the center's flagship Jaguar supercomputer has been doubled in power twice in the past year. In 2006 the system was taken from a peak performance of 26 trillion calculations per second (26 teraflops) to a peak performance of 54 teraflops. He said acceptance testing is currently under way for the system's latest upgrade, which will take it to a peak performance of more than 119 teraflops.

Bland explained that the system's peak performance will be more than doubled once again by early 2008. He said the center's next system, which will operate at a peak performance of 1,000 trillion calculations a second (1 petaflops), will be delivered by the end of 2008.

While each system upgrade offers researchers a substantial boost in computing power, Bland acknowledged that each also involves taking the system out of service for a time.

"I realize that is a great inconvenience to each and every one of you," he said, "but to some extent that is the price we pay for progress."

Researchers from a range of scientific fields used the meeting to outline their accomplishments and plans.

Lawrence Buja of the National Center for Atmospheric Research (NCAR) pointed to the increasing sophistication and confidence climate modelers have gained through the use of modern supercomputers. He said his group is especially looking forward to the petaflops supercomputer that will be coming to Oak Ridge.

“With the horsepower we will run more ensembles to greatly reduce the uncertainty of the answer,” he said. “Our own working-group plans heavily involve Oak Ridge.”

Buja presented several visualizations developed through the group’s Community Climate System Model. One showed temperatures across the globe increasing since 1870 and projected to 2100. The visualization included the effects of major volcanic eruptions such as Krakatau in 1883 and Pinatubo in 1991. Even considering the effects of these major eruptions, however, rising temperatures cannot be attributed solely to natural phenomena. Another visualization showed shrinking summer sea ice in the arctic projected through this century.

Buja noted that his team at NCAR and climate modeling in general gained credibility among policy makers and the public with the publication earlier this year of the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report. Much of the computer simulation for that report was produced on NCCS systems.

“The strength and the clarity of the message coming out of the IPCC process is directly related to the trust that we have in our model results,” he said. “In the past we knew the flaws. But this time around we were able to put much more realistic processes in almost every one of the components.”

The users meeting also allowed researchers to sharpen their supercomputing skills, with activities ranging from a visualization tutorial to a workshop on porting and optimizing their code for NCCS systems.

NCCS end-to-end solutions lead Scott Klasky worked with Mladen Vouk, Jeff Ligon, and Pierre Mouallem of North Carolina State University and Ilkay Altintas of the San Diego Supercomputing Center to present an especially well-received workshop on scientific-data workflow.

Scientific workflow systems allow for some automation in scientific-data management and analysis. These systems combine technologies and provide graphical user interfaces to help scientists increase their efficiency and focus on their science.

Users also had an opportunity to gather for a meeting of the NCCS Users Group. The group elected ORNL climate researcher John Drake as its chairman for the coming year and adopted an updated charter, which can be viewed on the NCCS Web site (www.nccs.gov).

Users Now Driving Upgraded Jaguar

Exciting performance seen for 119 teraflops system

Acceptance testing has been completed for the NCCS's upgraded Cray XT4 Jaguar supercomputer, with the system now able to perform up to 119 teraflops.

Jaguar now comprises 124 cabinets and 11,708 dual-core AMD Opteron™ processors. On average each cabinet houses 96 processors, and the system features 46 terabytes of memory and 750 terabytes of disk storage.

Acceptance testing involved running a number of science applications for many hours to put the machine through its paces. "We are excited about the performance that we see for a number of scientific applications," said LCF Director Buddy Bland. "For example, LSMS, a major materials code used for modeling semiconductors and storage devices, achieved 68% of the peak performance. We expect LSMS to achieve in excess of 80 teraflops sustained performance on the new system."

The upgraded system is the center's latest milestone as it pursues an aggressive schedule of upgrades. Jaguar will be upgraded once again by late 2007, reaching a peak performance of 250 teraflops as dual-core processors are replaced with AMD quad-core processors. The NCCS will take delivery of another system, one capable of 1 petaflops, by the end of 2008.

"With this expansion, the Department of Energy's Leadership Computing Facility at the National Center for Computational Sciences reaches another milestone along the path to a petaflops," said Thomas Zacharia, associate lab director. "Scientists from around the nation will be better able to tackle challenges using increasingly complex simulations that will provide new insights in a host of disciplines."

National Geographic Turns to NCCS Users

Astrophysicists explain exploding stars

NCCS astrophysics researchers Stan Woosley of the University of California–Santa Cruz and Adam Burrows of the University of Arizona were recently featured in *National Geographic* magazine.

The two were central to an article in the magazine's March issue entitled "Bang: The Cataclysmic Death of Stars." Besides quoting the two researchers, the article also included a supernova visualization from Woosley's project that was created from simulations run on the NCCS Jaguar supercomputer.

HPC Veteran to Lead NCCS Operations

Rogers brings experience from computing centers around the country

James H. Rogers has joined the NCCS as director of operations. He comes to the NCCS from Computer Sciences Corporation in Huntsville, Alabama, where he was a principal solutions architect.

Rogers has broad experience in HPC and has provided strategic-planning, technology-insertion, and integration support for multiple computing centers, including the U.S. Army Corps of Engineers Engineer Research and Development Center, the Aeronautical Systems Center, the National Aeronautics and Space Administration (NASA) Goddard Space Flight Center, the NASA Ames Research Center, the Defense Intelligence Agency, and the Alabama Supercomputer Center. He has also been part of the Supercomputing (SC) series of conferences, most recently as the executive director for SC05 and as a member of the SC Steering Committee.

Rogers will have primary responsibility for ensuring that the NCCS meets its commitments to the sponsors and users of the center by managing day-to-day operation of the NCCS systems and developing plans for future generations of systems and infrastructure.

He will take over these duties from Doug Kothe, who has been serving as NCCS acting director of operations as well as director of science. Kothe will now focus on his role as director of science.

Staffer Takes NCCS Message to Venerable Technical Society
Chattanooga Engineers Club founded in 1924

Bobby Whitten of the NCCS User Assistance and Outreach Group recently had the opportunity to tell one of the country's oldest technical societies about the center's work.

Whitten spoke to the Chattanooga Engineers Club, founded in 1924. He discussed the center's HPC systems and the cutting-edge science taking place at the NCCS.

Whitten visited the club through the ORNL Speakers Bureau. He noted that club members were especially interested in climate research being conducted at the NCCS, likely because of the recent report on global warming from the IPCC.

"They seemed to be as interested in the science as they were the machines. I got more questions involved with the machines; however, many of them were interested in what we were discovering about the climate. There seemed to be quite a few people that, I assume, have heard all the debates in the public recently about the climate."

Members were also interested in the ability of off-site users to gain access to Oak Ridge supercomputers, according to Ron Bailey, the group's vice president and a faculty member at the University of Tennessee–Chattanooga.

Bailey thanked Whitten for speaking to the group and said the presentation went over very well.

"It was well received," Bailey said. "He got good feedback from the club."