Conference

DOE at SC08

An estimated 10,000 members of the global high-performance computing community convened in Austin, Texas for the SC08 conference, and significant portions of the technical program represented knowledge and expertise developed by DOE national labs and programs.

The six-day Technical Program featured:

- Technical papers: of the 59 papers selected for the conference, 22 were written or co-authored by researchers at DOE national laboratories
- Tutorials: of the 25 full-day and half-day tutorials, 11 were organized and presented by DOE-supported scientists
- Panels: SC08 featured six panel sessions, five of which included DOE researchers
- Workshops: of the 13 workshops held in conjunction with SC08, five were led by researchers from DOE laboratories or DOE-supported projects

In the SC08 Exhibition, 13 DOE national laboratories showcased their leading-edge research and facilities. Researchers and staff from DOE labs and programs played key roles in planning, organizing, and conducting SC08. "Just as DOE provides significant leadership in the fields of scientific computing and networking, the expertise contributed by DOE researchers who have served on SC organizing committees over the years has been critical for the growth of the conference as the leading forum of the HPC community," said SC08 General Chair, Professor Patricia Teller. "From the exceptionally strong Technical Program to the conference network to critical organizational and communications support, SC08 has greatly benefited from the efforts by volunteers from DOE institutions."

National Science Foundation

Seidel Joins NSF

Edward Seidel, renowned astrophysicist and computational scientist, is the new director of the Office of Cyberinfrastructure for the National Science Foundation (NSF). "NSF's Office of Cyberinfrastructure is immensely important to all aspects of the science and engineering research the agency funds, and we're excited that a respected leader such as Dr. Seidel is able to join us," said NSF Director Arden L. Bement, Jr. in announcing Seidel's appointment.

Seidel joined the NSF from Louisiana State University (LSU), where he retains his position as a professor in the Departments of Physics & Astronomy and Computer Science and was also the founding director of the LSU Center for Computation & Technology. He had previously worked for seven years as a professor at the Max Planck Institute for Gravitational Physics (Albert Einstein Institute) in Potsdam, Germany, where he founded and led numerical relativity and e-science groups. Seidel also led the team that developed Cactus, an application initially designed to numerically solve Einstein's equations for general relativity and thus model black holes, neutron stars, and boson stars.

Large Hadron Collider

ESnet to Link LHC Data to U.S. Research Community

When hundreds of billions of protons, approaching the speed of light, collide in the Large Hadron Collider (LHC)—the energy release and particle explosions will be extraordinary. Scientists hope the remnants from these subatomic smashups will provide valuable insights into the origins of matter and dark energy in the Universe.

Across the globe, researchers will be anxiously awaiting the results of this experiment. They anticipate that over 40 million proton collisions per second will occur in the LHC, a gigantic particle accelerator spanning the French–Swiss border. This will generate more data than the international scientific community has ever tried to manage.

Fortunately, the physicists foresaw the looming data challenge and communicated it to engineers at the U.S. Department of Energy's Energy Sciences Network (ESnet). As a result, ESnet4 was developed, a new large-scale science data transport network with enough bandwidth to transport multiple 10 gigabits of information per second. For comparison, this capability is equivalent to transmitting 500 hours of digital music per second for each 10 gigabit line, if a minute-long MP3 file is about 2.4 megabits.

The LHC is the first experiment ever to utilize this network, which connects DOE national laboratories to researchers across the country. ESnet is funded by the DOE and managed by Lawrence Berkeley National Laboratory.

"ESnet4 is one of the most robust scientific data networks in existence," says Joseph Burrescia, General Manager for ESnet. "The science environment of today is very different from that of a few years ago. ESnet4 provides high-speed, highly reliable connectivity between laboratories and U.S. and international research institutions required to support the inherently collaborative, global nature of modern large-scale science."

Two detectors inside the LHC—ATLAS and CMS—will record the material spewing out of protons that are ripped apart by the violent collisions. Initially, these data will be stored at the European Organization for Nuclear Research, known by its French acronym, CERN, which manages the LHC. From CERN in Geneva, information will travel directly across the Atlantic Ocean via the USLHCnet, a reliable fiber optic network which can transfer data at the multiple gigabit-per-second rates produced by the experiment. This network is managed by researchers at the California Institute of Technology in Pasadena, California.

In the U.S. the Brookhaven National Laboratory in Upton, New York will process and store data collected by the ATLAS detector, and the Fermi National Accelerator Laboratory in Batavia, Illinois will do the same for CMS data. Researchers at universities across the country, many of which are connected by Internet2, a leading research and education network, will be able to connect to these datasets through ESnet4. Two years ago, ESnet and Internet2 launched a partnership to develop and deploy DOE's next-generation scientific network.

"LHC is just the beginning. ESnet4's innovative and reliable infrastructure allows scientists from all over the world, and across disciplines, to exchange large datasets and analyses efficiently. It is these collaborations, this sharing of information, that allows us to better understand the world around us," said Burrescia.

National Laboratories

LLNL's Steven Ashby Joins PNNL as Deputy Director for Science and Technology

Steven Ashby has joined Pacific Northwest National Laboratory (PNNL) as the new Deputy Director for Science and Technology (DDST) after a distinguished career at Lawrence Livermore National Laboratory (LLNL). As the DDST, Ashby will work with PNNL's scientific and technical staff to advance its S&T capabilities on behalf of scientific discovery, energy independence, environmental stewardship, and national security.

"One of my main objectives is to determine how we can best integrate our current science and technology programs to enable new discoveries and to address national needs, especially in energy and security," Ashby said. "As I learn more about PNNL's strengths in all areas, the goal will be to leverage those strengths through partnerships with other laboratories and universities to make the biggest possible impact for the nation."

Ashby, who is well known in the computational science community, is particularly enthusiastic about working with colleagues at PNNL in developing a comprehensive computing strategy for the Laboratory.

"Our computational science capabilities are very strong, but they may not be as well known as those at other labs," Ashby said. "We will be looking to see how the pieces here can work together to create a program that is greater than the sum of the parts."

Ashby points to the NWChem chemistry code and a suite of subsurface science applications as examples of PNNL's expertise in computational science. In his view, they also represent an opportunity for PNNL to collaborate with others in the spirit of SciDAC.

PNNL

Steven Ashby

"NWChem is today's leading computational chemistry code. We want to take it to the next level of performance to take full advantage of the next generation extreme-scale computing systems," Ashby said. "Subsurface science codes, which I first learned about as a graduate student, have exploited parallel supercomputing power for years in support of important DOE programmatic work. PNNL is investing internally in designing implementation of both of these capabilities so that they can be effectively used for extreme-scale problems and we recognize that we will need to engage the SciDAC community in doing this."

PNNL has earned a strong international reputation in the area of data science through its work in information visualization and analytics for national security programs. "Though not as well known in the science community, these efforts are world class and we plan to bring them to bear on computational science projects of interest to the SciDAC community."

As an example of how this expertise can be applied to DOE needs, Ashby noted that a team at PNNL developed ScalaBLAST, a parallel version of the BLAST code being used for high-performance data-intensive bioinformatics analysis at DOE's Joint Genome Institute (JGI) in California. The new code scales up to thousands of processors and is already improving JGI's productivity.

A key element of PNNL's computing landscape is its hardware, primarily Chinook, a 160 teraflop HP system in EMSL, the Environmental Molecular Sciences Laboratory, a user facility for DOE's Office of Biological and Environmental Research. EMSL houses one of four DOE computing centers running large-scale, high-impact computational science applications under INCITE, the Innovative and Novel Computational Impact on Theory and Experiment program. PNNL has also installed a Cray XMT system featuring massively multithreaded architecture as part of the Center for Adapative Supercomputing Software focused on Multithreaded Architectures (CASS-MT). "Our next challenge is to determine how best to apply these tremendous resources," Ashby said, "to areas of greatest importance to DOE and the nation."

Prior to joining PNNL, Ashby spent nearly 21 years at LLNL, where he conducted numerical algorithms research and led the ParFlow groundwater modeling project. He also founded the Center for Applied Scientific Computing and served as leader of the Computing Applications and Research Department. He remains active in the computational science community through his involvement in OASCR and SIAM activities.

Workshop

AMR08 Explores Major Areas in Applied Mathematics

Researchers from throughout the United States met at Argonne National Laboratory October 15–17 to participate in a workshop on Applied Mathematics Research. The workshop, popularly known as AMR08, provided a forum for participants to exchange technical information in four areas: linear and nonlinear systems, multiscale phenomena, uncertainty quantification and sensitivity analysis, and optimization of complex systems.

The meeting featured plenary talks from researchers and agency managers, including Weinan E (multiscale modeling, Princeton University), Inez Fung (climate modeling, University of California–Berkeley), Alexander Gray (large-scale data analysis, Georgia Tech), Fred Johnson (DOE), David Keyes (petascale methods for energy applications, Columbia University), and Karen Willcox (uncertainty quantification and optimization of complex systems, MIT).

Topics ranged from computational mathematics technology and scalable software to their application in advanced climate modeling and astrophysics simulations. Breakout sessions and poster sessions provided ample time for researchers to discuss recent advances, major challenges, and new approaches and tools. Friday included a plenary presentation by David Brown (Lawrence Livermore National Laboratory) on future directions for applied mathematics. Tours of the Advanced Photon Source and the Argonne Leadership Computing Facility concluded the meeting on Friday afternoon.

Funding for AMR08 was provided by the DOE Office of Advanced Scientific Computing Research's Applied Mathematics Program, under the direction of Dr. Homer Walker. The organizing committee comprised researchers from eight national laboratories and three U.S. universities and was chaired by Jorge Moré of Argonne National Laboratory.