NERSC NEWS
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER
NOVEMBER 2007

New Director for NERSC

Kathy Yelick, a professor of computer science at the University of California at Berkeley and an internationally recognized expert in developing methods to advance the use of supercomputers, has been named director of NERSC.

Yelick has received a number of research and teaching awards and is the author or co-author of two books and more than 75 refereed technical papers. She earned her Ph.D. in computer science from MIT and has been a professor at UC Berkeley since 1991 with a joint research appointment at Berkeley Lab since 1996.

"We are truly delighted to have Kathy serve as the next director of NERSC, and only the fifth director since the center was established in 1974," said Berkeley Lab Director Steven Chu. "Her experience and expertise in advancing the state of high performance computing make her the perfect choice to maintain NERSC's leadership position among the world's supercomputing centers."

Yelick will officially assume her new job in January 2008. Yelick, who has been head of the Future Technologies Group at Berkeley Lab since 2005, succeeds Horst Simon as head of NERSC. Simon, who has led NERSC since 1996, will continue to serve as Berkeley Lab's Associate Director for Computing Sciences and Director of the Computational Research Division.

Kathy Yelick

"When Horst Simon announced that he wanted to relinquish the leadership of NERSC, we knew he would be a tough act to follow," said Michael Strayer, head of DOE's Office of Advanced Scientific

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Model Comparisons

FUSION RESEARCH GROUP PUBLISHED SEVERAL RECENT PAPERS EXAMINING THE RESULTS OF TWO TYPES OF TURBULENCE SIMULATIONS AND THEIR IMPACT ON TOKAMAK DESIGNS

Scientists from the Advanced Plasma Microturbulence Project have published several papers recently that show how they resolve the significant differences between two types of electron temperature gradient (ETG) turbulence simulations in fusion research.

The researchers have been running simulations at NERSC using particle-in-cell (PIC) and continuum gyrokinetic codes in order to reconcile the large gap of electron thermal conductivity values between the two types of simulations. Investigating the discrepancy is important in understanding electron heat transport during fusion energy generation, when a strong electric current heats and confines a hot plasma in a magnetic field inside a tokamak. The tokamak is a donut-shaped device and a leading design for making fusion power feasible.

The goal of the project is to develop precise models of ETG drift-wave turbu-

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Head of the Class

A CRAY XT4 NAMED FRANKLIN PASSES A RIGOROUS TEST AND BECOMES AN OFFICIAL MEMBER OF THE NERSC SUPERCOMPUTING FAMILY

NERSC and Cray recently announced the successful completion of the acceptance test of one of the world's largest supercomputers. The powerful Cray XT4™ system contains nearly 20,000 processor cores and has a top processing speed of more than 100 teraflops.

The next-generation supercomputer will be used to advance a broad range of scientific research. Named "Franklin" in honor of the first internationally recognized American scientist, Benjamin Franklin, the Cray XT4 system enables researchers to tackle the most challenging problems in science by conducting more frequent and increasingly detailed simulations and analyses of massive sets of data.

"With Franklin, we are increasing the computational power available to our 2,900 NERSC users by a factor of six, providing them with access to one of the world's fastest supercomputers dedicated to open scientific research," said Michael Strayer, associate director of DOE's Office of Advanced Scientific Computing Research, which funds NERSC. "We have high expectations that NERSC's proven track record of scientific productivity will provide many new discoveries and understandings."

The highly scalable Cray XT4 system is capable of running applications across a wide range of scientific disciplines, including astrophysics, fusion, climate change prediction, combustion, energy and biology. Franklin will enable researchers at Berkeley Lab to address such problems as developing better models of the Earth's climate and using it to predict the impact of carbon dioxide emissions and global warming. The powerful system will also allow researchers to explore clean energy technologies and validate theories that attempt to uncover evidence that explains the origin of the universe.

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Franklin Good to Go *continued from page 1*

"Our new Cray XT4 system has demonstrated that it can deliver a high sustained performance on a demanding scientific workload in a rigorous production environment while at the same time permitting users to explore scaling to 20,000 cores," said Horst Simon, NERSC Director. "NERSC is proud to accept one of the largest 'broad impact science' supercomputers in the world for its demanding user community."

Franklin has a theoretical peak speed in excess of 100 teraflops (100 trillion floating point operations per second). In assessing proposed systems, the Cray XT4 scalable architecture promised to deliver high sustained performance, which is critical to NERSC's 24x7 operation to meet users' supercomputing demands.

"We are very excited to see one of the largest supercomputers in the world opened up to the expansive user community at NERSC," said Peter Ungaro, president and CEO of Cray. "The Cray XT4 system will provide the computational power to enable researchers who compute at NERSC to efficiently tackle some of the most important problems we face today. With high sustained performance, scalability and upgradeability to petaflops capacity as its key attributes, the Cray XT4 supercomputer will help enable major advances in a number of scientific fields now and in the future."

As part of an extensive testing program, a number of NERSC users were given early access to Franklin to ensure that the system could handle the most demanding scientific applications.

"I am extremely impressed with Franklin," said Robert Harkness, an astrophysicist at the San Diego Supercomputer Center working on a project aimed at precisely measuring the cosmological parameters that describe the shape, matter-energy contents, and expansion history of the universe. Running an application called ENZO, the project seeks to increase our understanding of the dark energy and dark matter thought to make up more than nine-tenths of the universe. "We have run the largest instances of ENZO ever, anywhere, and found that the performance and scaling on Franklin are both strong and better than other computer platforms we have used at other computing centers."

Another project, led by Julian Borrill of Berkeley Lab, leveraged Franklin's computing power to prepare for analyzing the massive amounts of data to be sent back to Earth by the Planck satellite, set for launch in 2008. A joint U.S.-European project, Planck will use 74 detectors to measure the cosmic microwave background, the residual radiation from the actual "Big Bang." Last scattered some 400,000 years after the Big Bang, it provides the earliest possible image of the universe, including encoded signatures of the fundamental parameters of all matter.

"I am delighted to report that we have just successfully created a map of the entire Planck Full Focal Plane one-year simulation," Borrill said. "This is the first time that so many data samples — three terabytes of data in 50,000 files, representing all the information collected by Planck during one mission year — have been analyzed simultaneously, a primary goal of our group's early Franklin efforts."

Franklin contains 9,672 AMD dual-core Opteron 2.6 GHz processors with 39 terabytes of memory. Running on 16,384 processor cores, the group was able to complete the run in just 45 minutes.

During negotiations to procure the system, NERSC and Cray mapped out a plan to install the Cray Linux Environment (CLE) on each of Franklin's 9,672 nodes. As a result of this partnership, NERSC became the first center with a production XT4 running CLE, an ultra-lightweight version of the standard Linux operating system. CLE makes the system easier to use, allowing users to more easily port their scientific applications from other architectures. During extensive testing, about 300 different features and functions were tested and validated, making CLE more reliable with the same or better performance than previous XT operating systems.

Franklin wouldn't have passed the acceptance test without the hard work put in by the NERSC staff to troubleshoot hardware and software problems that are typical of getting a supercomputer to work properly, especially for demanding, large-scale scientific research.

Working closely with early users and using their feedback to resolve any issues was key to prepare Franklin for the test.

"One of the biggest issues was to get Franklin's reliability up to the levels that

Hard work by NERSC and Cray staff has paid off. The new Cray XT4, named Franklin, recently completed the acceptance test, making it available for scientists in a wide range of disciplines.

NERSC users expect," said Jonathan Carter, head of the User Services Group at NERSC. "Part of this was handled by soliciting early user feedback and reporting problems to Cray quickly. Another part was keeping the composite metrics like job failure rates, SSP and ESP high on the list of things Cray needed to pay attention to."

Helen He, a member of the User Services Group, added: "The early users got a lot of useful work done. Many were able to run high-concurrency jobs to tackle much larger problems and model resolutions that were impossible before."

Here is a list of people who worked on getting Franklin to NERSC:

Procurement team: Bill Kramer, Lynn Rippe, Jonathan Carter, Nick Cardo, David Skinner, Brent Draney, Erich Strohmaier, Liz Ciabetta.

Negotiation team: Bill Kramer, Lynn Rippe, Jonathan Carter, Nick Cardo, Brent Draney, Jim Craw.

Implementation team: Bill Kramer, Lynn Rippe, Jonathan Carter, Nick Cardo, Helen He, Harvey Wasserman, Jim Craw, Howard Walter.

Learn more about Franklin at http://www. nersc.gov/nusers/systems/franklin.

Kathy Yelick

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Computing Research, which funds NERSC. "But with the selection of Kathy Yelick as the next director, I believe that NERSC will continue to build upon its success in advancing scientific discovery through computation. We are extremely happy to have her take on this role."

In 2006, Yelick was named one of 16 "People to Watch in 2006" by the newsletter HPCwire. The editors noted that "Her multi-faceted research goal is to develop techniques for obtaining high performance on a wide range of computational platforms, all while easing the programming effort required to achieve high performance. Her current work has shown that global address space languages like UPC and Titanium offer serious opportunities in both productivity and performance, and that these languages can be ubiquitous on parallel machines without excessive investments in compiler technology."

In addition to high performance languages, Yelick has worked on parallel algorithms, numerical libraries, computer architecture, communication libraries, and I/O systems. Her work on numerical libraries includes self-tuning libraries which automatically adapt the code to machine properties. She is also a consumer of parallel systems, having worked directly with interdisciplinary teams on application scaling, and her own applications work includes parallelization of a CFD model for blood flow in the heart. She is involved in an NCR study investigating the impact of the multicore revolution across computing domains, and was a co-author of a Berkeley study on this subject known as the "Berkeley View." Yelick speaks extensively on her research, with over 15 invited talks and keynote speeches over the past three years.

"After working on projects aimed at making HPC systems easier to use, I'm looking forward to helping NERSC's scientific users make the most effective use of our resources," Yelick said. "NERSC has a strong track record in providing critical computing support for a number of scientific breakthroughs and building on those successes makes this an exciting opportunity."

Read an overview of Yelick's research here or see her UC Berkeley home page.

SPOTLIGHT

VISIT FROM STUTTGART COMPUTING CENTER DELEGATION

Wolfram Ressel

Wolfram Ressel, Rector of the University of Stuttgart, and three senior representatives of the High Performance Computing Center Stuttgart (HLRS), visited Lawrence Berkeley National Laboratory and NERSC in October. The visitors were particularly interested in energy-efficient architectural designs being drawn up for Berkeley Lab's planned Computational Research and Theory facility, which will house both NERSC and the Computational Research Division. It will also serve and promote a closer tie with researchers from UC Berkeley.

The HLRS is currently housed in a small building and is interested in designing a new facility. Because electricity in Germany costs nearly four times as much as in California, the group engaged in extensive discussions about LBNL efforts to design more efficient buildings as well as a project to develop new computer designs which use less power. After a morning of talks, the visit concluded with a tour of the NERSC Center at the Oakland Scientific Facility.

NERSC ON TV

Bill Tschudi

An ABC station in the Bay Area featured NERSC in a story about building energy-efficient supercomputer centers at research institutions and businesses. The story, which appeared on Nov. 5, called NERSC "one of the world's most efficient" supercomputing centers.

The story, called "The Next Step in Computer Powering," focused on efforts by researchers to develop better technologies for cooling supercomputers. The exploration will not only benefit scientists who use powerful computers for their work, it also will help businesses that rely on buildings full of servers to process and store data. Large companies such as Google have been setting up data farms in parts of the country that promise cheap electricity.

It highlighted the work by Bill Tschudi from Berkeley Lab's Environmental Energy Technologies Division. Tschudi uses NERSC as a test site for his research.

Tsuchudi and his research team have been testing different cooling methods, including the use of DC instead of AC power.

You can read the story and watch the video at the KGO-TV site.

CHAT WITH EXPERTS AT SC07

Berkeley Lab researchers will hold talks at the Lab's SC07 booth from Nov. 13 to Nov. 15. Thirteen researchers will present a wide range of discussions, including scientific data management, power-efficient computing, dynamic virtual circuits and visualization.

The presentations provide a good opportunity to learn about trends in computer science and computational research, as well as key issues in operating a supercomputer center and national science network.

The speakers include George Smoot, winner of the 2006 Nobel Prize in Physics, who will discuss computational cosmology.

The Berkeley Lab booth is located at #351. You can find the research talk schedule at http://www.lbl.gov/CS/Archive/BerkeleyLabTalksSC07.pdf

Fusion Research

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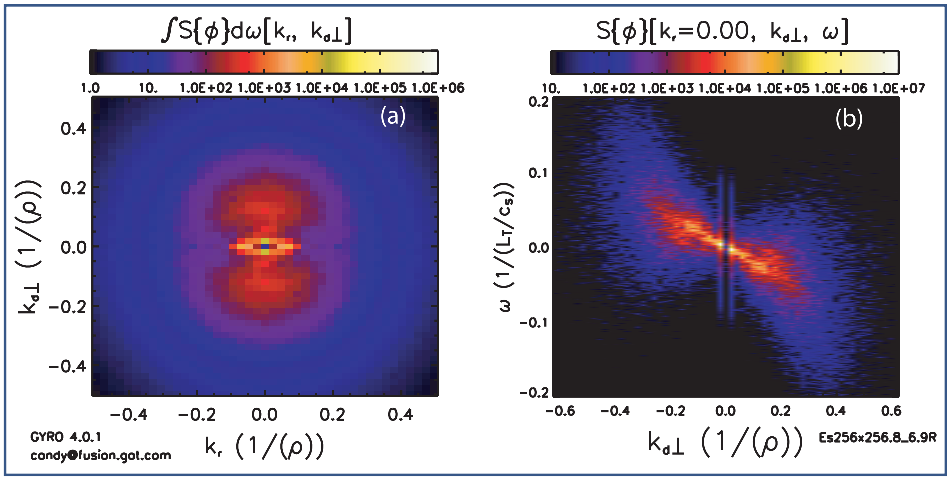
lence using three-dimensional kinetic and fluid simulations. Figuring out drift-wave instabilities and controlling them has improved plasma energy confinement in tokamak experiments.

Headed by William Nevins of the Lawrence Livermore National Laboratory, the project has pooled together the expertise from many institutions. Those researchers are Andris Dimits, Bruce Cohen and Dana Shumaker at Livermore Lab; Greg Hammett at the Princeton Plasma Physics Laboratory; William Dorland at the University of Maryland; Ronald Waltz, Jeff Candy and Jon Kinsey at General Atomics; and Frank Jenko at the Max Planck Institut für Plasmaphysik (IPP) in Garching, Germany.

"NERSC's machines and support infrastructure are most hospitable for getting our work done," Cohen said.

The researchers have published several papers this year chronicling how they have tackled several vexing questions about the simulation codes and their diverging results. Previously published results of ETG turbulence simulations that used gyrokinetic continuum codes produced large values of the electron thermal conductivity, which could make ETG turbulence a significant force to consider for tokamak design and operation. But those results were thrown into question when more recent particle-in-cell simulations yielded much lower thermal conductivity values.

In a paper published in Physics of Plasmas in August, Nevins and his fellow researchers demonstrated that GEM (developed by Scott Parker and Yang Chen at the University of Colorado), a turbulence simulation code using the particle-in-cell method, would produce substantially the same results at the same operating point as popular continuum and particle-in-cell codes such as GYRO, GS2, GENE and PG3EQ.



Fluctuation spectrum of electron temperature gradient turbulence projected into (a) the (k_r, k_perp) plane, and (b) the (k_perp, omega) plane. At small k_perp the fluctuation spectrum is anisotropic with a well-defined frequency at each k_perp, while at large k_perp the spectrum becomes isotropic with no well defined frequency.

The authors noted that verifying the codes is an important step in accurately modeling how plasma behaves in a tokamak. "Benchmarking turbulence simulation codes is an important exercise in code verification. This code verification exercise is particularly important in light of recent controversies, in which particle and continuum codes showed qualitative differences in electron energy flux," the researchers wrote. The paper can be found here.

In other papers, published in Physics of Plasmas in December 2005, and in Nuclear Fusion in July 2007, the scientists showed that discrete particle noise was the cause of the lower thermal conductivity values. In those previously published results, the particle noise would suppress the turbulence, skewing the models. Their findings corroborated other studies showing that particle-in-cell simulations could produce higher thermal conductivity values "provided that care is taken to monitor and manage the simulation noise."

The research further supported earlier conclusions from continuum-code simulations that the values of the thermal conductivity are large enough to play a significant role in tokamaks. Read the paper here.

In a third paper, which was published in the August issue of Plasma Physics and Controlled Fusion, the researchers followed up their previous simulation work using GYRO, a continuum code. In 2006, they had established a connection between velocity space resolution, entropy saturation and conservation, and numerical dissipation. This year, they found that ETG simulations with kinetic ions could cure unphysically large saturation levels in ETG simulations with adiabatic ions. You can read the abstract of the paper here.

Learn more about the fusion project at http://www.mfescience.org.

WHAT IS NERSC NEWS?

NERSC News publishes every other month and highlights the cutting-edge research performed using the National Energy Research Scientific Computing Center, the flagship supercomputer facility for DOE's Office of Science. NERSC News editor Ucilia Wang can be reached at 510 945-2402 or Uwang@lbl.gov. Find previous NERSC News articles at http://www.nersc.gov/news/nerscnews.