National Center for Computational Sciences Snapshot
The Week of March 16, 2009

Zacharia Takes Science and Technology Posts

Nichols named interim associate laboratory director for computing at ORNL

Thomas Zacharia, Oak Ridge National Laboratory's (ORNL's) associate director for computing and computational sciences, has been named ORNL deputy laboratory director for science and technology (S&T) and UT-Battelle senior vice president for S&T, responsible for coordinating ORNL's major research and development (R&D) programs.

As deputy lab director, Zacharia will oversee one of the nation's largest R&D programs, with annual expenditures in excess of $1.3 billion in materials and physical sciences, energy and engineering sciences, computational sciences, life and environmental sciences, neutron sciences and national security. His appointment becomes effective April 1.

"Thomas has done a remarkable job of building ORNL's computational program into one of the world's best," said ORNL Director Thom Mason. Under Zacharia's leadership, in November 2008 "Jaguar," a Cray XT supercomputer at ORNL's computing complex, became the world's fastest supercomputer for open science. Simulations on Jaguar help the nation's scientists explore grand challenges in science and engineering, such as developing new energy solutions and better understanding climate change.

Zacharia's appointment is part of a strategic reorganization of resources as the national lab positions itself to make the most of an historic investment of funds for transformational scientific research by the President and Congress. The recently enacted fiscal year 2009 Omnibus Bill and the Stimulus package together contain more than $2.3 billion in increased spending for U.S. Department of Energy (DOE) Office of Science programs. ORNL, managed by UT-Battelle for DOE, is poised to hire 1,000 employees in the next two years, according to Mason.

ORNL's Jeff Nichols will assume the position of interim associate laboratory director for computing and computational sciences while an international search is conducted for Zacharia's replacement. Nichols currently serves as the deputy associate laboratory director of ORNL's Computing and Computational Sciences Directorate, where he leads efforts to build, install and deploy next-generation supercomputers for DOE, the National Science Foundation, and the Department of Defense.

Previously Nichols led the Computer Science and Mathematics Division at ORNL and the Environmental Molecular Sciences Laboratory at DOE's Pacific Northwest National Laboratory, where high priority was given to the development, deployment and use of scalable computational science community codes to solve grand-challenge problems crucial to the nation.

Modeling the Weather's Extreme Mood Swings

Climate scientists look to the past to prepare for the future

Weather is not always kind. Tropical storms, blizzards, and other weather "mood swings" are some of the more temperamental traits of a climate's personality.

Researchers at the Oak Ridge National Laboratory Leadership Computing Facility are using the world's fastest supercomputer for open scientific research to recreate the last century's global climate and examine some of its more destructive weather tantrums. By understanding the past, scientists may be able to more accurately predict future extreme weather under climate change.

"We can represent the weather for every extreme event in the historical record for which we have observations," said Gilbert Compo of the University of Colorado, principal investigator of the Surface Input Reanalysis for Climate Applications (SIRCA) project.

To confidently project weather extremes into the twenty-first century, it is necessary to make sure daily data from the nineteenth and twentieth centuries are accurately reflected, Compo explained.

The SIRCA project is conducted under the auspices of the Cooperative Institution for Research in the Environmental Sciences Climate Diagnostics Center of the University of Colorado and the National Oceanic and Atmospheric Administration Earth System Research Laboratory. As part of the project, researchers are reconstructing global weather conditions in six-hour intervals from 1850 to the present. An international initiative called Atmospheric Circulation Reconstructions over the Earth facilitates collection of more observations for the project and their applications.

Compo and his team expect the results of the SIRCA project will help scientists better understand extreme weather throughout recent history. "The datasets should be good for looking at extreme events like colder outbreaks and heat waves," Compo said.

Some major climate events of the nineteenth and twentieth centuries had tragic consequences, and scientists hope to better anticipate future trends with the help of historical simulations.

Three million Americans fled from the Great Plains during the 1930s Dust Bowl, when dust storms rolling over the plains left half a million people homeless. Dust clouds picked up the dry soil of fields left barren by drought. The dust was thick enough to clog lungs and cause a condition known as dust pneumonia that killed hundreds.

Another weather tantrum was the Children's Blizzard in January 1888, which killed 200 people on the Great Plains who were exposed to the subzero temperatures and blasts of snow. Half of the victims were children trying to get home from school during the blizzard.

Compo also expects to follow the warming trend seen in the Arctic from the 1920s to the 1940s. By effectively tracking droughts, storms, and other highs and lows of the past, he thinks improvements can be made to current climate models, which are expected to predict similar extremes in the future.

The climate model for the SIRCA project will be run on the Department of Energy's Jaguar supercomputer at ORNL. Initial datasets from SIRCA's predecessor, the 20th Century Reanalysis Project, are reconstructing global climate and weather from the 1870s to the present. Scientists expect that project to be completed this fall. SIRCA is projected to extend the team's reconstructions from the 1870s back to the 1850s at a spatial resolution two times higher than the Century Reanalysis by fall 2012.

The SIRCA and Century Reanalysis projects are the first of a three-phase reanalysis undertaking enabled by the Innovative and Novel Computational Impact on Theory and Experiment program. The task will map weather conditions in the troposphere and stratosphere, the lowest portions of the Earth's atmosphere.

It takes a lot of computer power to reconstruct a century and a half of weather. "To generate the 1850 to 2011 dataset, we expect to need 60 million [processing] hours," Compo said. "Without the supercomputer we couldn't do [the SIRCA study] at all."

Not only will researchers make forecasts for every six-hour period, requiring the use of hundreds of processors, but they will also make 56 forecasts for each period.

"Think of a newspaper weather map with the highs and lows for the day," Compo said. "It's like having 56 maps."

The SIRCA "weather maps" discern details of the Earth's surface as close as 100 kilometers apart. Compo and his team plan to zoom in on hurricanes, severe storms, and floods. For these extreme events, the computer will generate maps showing details 60 kilometers apart. Zooming on these details will require 100 times the computing power of the other weather maps.

An algorithm called the Ensemble Kalman Filter pulls this collection of datasets—or ensemble—into a single reconstruction that is closest to the actual weather conditions. The computer algorithm recasts the observational data into three-dimensional datasets of past weather conditions.

"In traditional numerical weather predictions, you combine the observations you have with a single numeric model integration," Compo said.

What comes first, observational data or the algorithm used to generate new forecasts? "It's a chicken and the egg issue," Compo said. "We combine the forecast with observations to change the forecast to be more consistent."

Consistency is key in climate modeling. Predictions of weather extremes require reliable computer modeling simulations, which help ensure future mood swings won't take us by surprise.

NCCS Science Seminars Tackle Research Needing Petascale Power

Scientists share simulation tips with research community

The National Center for Computational Sciences (NCCS) has resumed its monthly seminar series featuring speakers in sciences that would benefit from simulating research problems on the XT4/XT5 Jaguar supercomputer. Guest speakers are typically researchers in the computational sciences fields from outside the NCCS who collaborate with the center's staff and may use its Leadership Computing Facility, recently upgraded to 1.64 petaflops.

Dr. Balint Joo, a physicist in lattice quantum chromodynamics (QCD) at Thomas Jefferson National Accelerator Facility in Newport News, Virginia, gave the first presentation in the series on March 2, 2009. QCD is a mathematical theory that describes how the fundamental particles known as quarks and gluons interact to form nuclei and nuclear forces. Because the equations of QCD are not easily dealt with mathematically, they are often studied numerically using supercomputers, assuming a simplified world in which the particles move on a lattice of points in space and time. Joo discussed the computational technology behind lattice QCD, including gauge generation algorithms, software, and performance issues on the Cray XT computers at the NCCS and National Institute for Computational Sciences (NICS).

On March 10, Dr. Cecilia Bitz, professor of atmospheric sciences at the University of Washington and an affiliate physicist at the Polar Science Center, discussed her modeling of Arctic summer sea ice through the twenty-first century using the Community Climate System Model . Bitz showed that her modeling of summer ice loss does not support recent warnings that a permanently ice-free Arctic is imminent. While there was an anomalously large loss of summer ice in 2007, a phenomenon which is nonexistent in preindustrial models, such a loss occurs in twenty-first century models only 1 percent of the time, she said. However, under more pessimistic greenhouse warming scenarios, summer ice loss will occur with increasing frequency. Bitz said that future Arctic ice modeling coupled with atmospheric and oceanic studies should improve the predictive accuracy of the simulations.

The seminars are held in Room 128 (Lecture Hall), Building 5100, on the ORNL campus. Questions and suggestions for speakers for the seminar series may be directed to Ricky

Kendall (kendallra@ornl.gov). Information on the developing series is posted at http://www.nccs.gov/user-support/training-education/nccs-seminar-series/.

Videos of the seminars can be viewed at http://www.nccs.gov/category/podcast/ . Or interested parties can subscribe to the podcast via RSS feed from the NCCS website or on iTunes by searching for NCCS.

University Profs, Students Win Access to Computing Resources, Staff at NCCS

First-ever winners of ORAU/ORNL research competition

Four university professors and their students received $25,000 high-performance computing awards in February as winners in the first-ever computational research competition established by Oak Ridge Associated Universities (ORAU) and ORNL.

The grants, which are open to ORAU member universities, give faculty and student teams unique access to the NCCS's computing resources and staff. The $25,000 award, provided by ORAU for one year, may be extended for an additional two years for a total of $75,000. The first grants in this program came as the NCCS upgraded its Cray XT4 Jaguar to a 1.64 petaflops XT5 machine.

Shaikh Ahmed, an assistant professor in the Electrical and Computer Engineering Department at Southern Illinois University at Carbondale, and his students will work on the modeling and simulation of nanoelectronic devices. Yongmei Wang, an associate professor in the Chemistry Department at the University of Memphis, and students Jesse Ziebarth and Aaron Masur will use AMBER molecular dynamic software to model gene delivery, one of the steps necessary in gene therapy, which introduces foreign DNA into a host cell. Ming Ye, an assistant professor in the Scientific Computing Department at Florida State University, and student Geoffery Miller will develop software to assess the predictive uncertainty of contaminant transport and chemical reactivity in groundwater. Oleg Zikanov, an associate professor in the Mechanical Engineering Department at the University of Michigan, and his students will conduct computational studies in materials science.

"These grant recipients are among the first researchers in the world to have access to petascale supercomputing capabilities," said ORNL Director Thom Mason. "We look forward to the scientific discoveries that will emerge from the work that they and others do at ORNL."

"The funding that ORAU is providing helps enable outstanding university researchers to have access to ORNL's staff and impressive supercomputing capabilities to significantly advance their research endeavors," said Homer Fisher, interim ORAU president.

Proposals were chosen for their scientific importance and alignment with the laboratory's cross-cutting science agenda, the individual institutions' research goals, the faculty-student approach, and the qualifications of the faculty members. The researchers and their students will be able to begin their work at the NCCS as early as this summer.

Students Engage in Science Research Online

ORNL connects K–12 students with breakthrough science research

Participating in scientific research does not necessarily require a college degree. SciEdTech (http://sciedtech.org), a new outreach and science website, aims to bring tomorrow's science to today's kindergarten through twelfth-grade students.
"We're working on real-life science challenges of today and tomorrow, and we're computing at scales that are very unique," said Ross Toedte of the NCCS's visualization task group. "We can [provide] science lessons based on these problems."

The project's partners include researchers and educators from the NCCS and NICS, both located at the ORNL petascale computing complex, and ORAU.

While research institutions traditionally start interacting with potential future scientists as they progress through college, the goal of SciEdTech is to engage the scientific curiosity of younger students and their teachers.

"K–12 is an underrepresented portion of the education pipeline for ORNL," said Toedte.

Visualizations of data from simulations done on ORNL supercomputers will be designed for the website to teach basic science concepts to students as well as introduce them to the kinds of projects ORNL scientists are working on. Topics in astrophysics, climate change, biological processes, and nanotechnology are just a few of those being researched with the help of ORNL's supercomputer that will be represented on the site.

Students and teachers will be able to ask questions, post comments, and access other online resources to enhance classroom learning.

"We're starting to engage science teachers to tell us what infrastructure they use in their schools and what is the best way to deploy computational science in the classroom," said Toedte.

Marie Westfall, ORAU group manager, said that teachers are asking questions like "How do I quickly get what I need to energize and educate my students?"

Although still in its early stages, the website already provides information for students about upcoming science programs, such as the Tennessee Science Bowl. Likewise, teachers can get details about math- and science-education workshops.

“A teacher’s time is limited,” Westfall said. “This is a clearinghouse of things that do work and are categorized.”