

U.S. Department of Energy

New DOE Leadership is Strong on Science and Computing

With the new administration in office, the U.S. Department of Energy (DOE) has been given a new set of leaders that are highly recognized scientists. The new Secretary of Energy, Dr. Steve Chu (figure 1) holds a Nobel Prize in Physics for his research in cooling and trapping atoms with laser light. Fresh from his position as director of Lawrence Berkeley National Laboratory, Dr. Chu is also a strong proponent of computational science: "In areas where we can do experiments, computation lets you look at a level where our instrumentation doesn't allow us to look, or at the quantum level, which we could not measure directly, or in a molecular dynamics experiment, where we still don't have the ability to look at atomistic details, but simulation and modeling can help us see what is happening," ("Science, Computation, and Collaboration at Berkeley Lab," *SciDAC Review* 7, Spring 2008, p6).

The new Undersecretary for Science, Dr. Steven Koonin, is a theoretical physicist who also has a strong interest in computational physics. With experience at BP and CalTech, Dr. Koonin is also a past recipient of the E.O. Lawrence award.

Serving as the new director of the Office of Science is Dr. William F. Brinkman, another



Figure 1. Dr. Steve Chu.

researcher with an impressive physics background. Dr. Brinkman's experience includes positions at Princeton University, Bell Laboratories, Lucent Technologies, and Sandia National Laboratories.

Advanced Networking Initiative

Stimulus to Fund Advanced Networking Initiative

The Advanced Networking Initiative (ANI) plans to accelerate by several years the commercialization of 100 Gigabit per second (Gbps) networking technologies by deploying a demonstration national network prototype and conducting research and development on an advanced network testbed facility.

The prototype national network will span at least four distinct geographic regions, covering the three major Advanced Scientific Computing Research (ASCR) computing facilities and the New York multi-agency peering point providing transatlantic Research and Education (R&E) connectivity. This effort will validate prototype technologies for future deployment within the cutting-edge Energy Sciences Network (ESnet).

The prototype 100 Gbps network will be complemented by a testbed enabling enhanced research efforts on network management and critical control plane issues for optical networks. This effort is anticipated to lead the way in defining the optical control plane necessary to provision sub-wavelength point-to-point circuits in addition to exploring the challenges associated with end-to-end data transfers in excess of 10 Gbps.

The majority of the project funds will be distributed to Lawrence Berkeley National Laboratory through an existing contract. These funds will be distributed through established normal funding channels. New, competitively-awarded financial assistance agreements will be issued to scientists and researchers in academia and industry.

Argonne Leadership Computing Facility

ALCF Offers "Leap to Petascale" Workshop

INCITE users, are you ready to run your research project on 40 racks of the Blue Gene/P? Then attend "Leap to Petascale" on May 27–29, a workshop being held at the Argonne Leadership Computing Facility (ALCF). Users will learn about the ALCF and the petascale resources available to them. Then, ALCF performance engineers will help users scale and tune their applications on the 40 racks. Attendees must have ported their code to at least one rack of the Blue Gene/P and must have a current account with the ALCF. This is an especially good opportunity for anyone considering applying for a 2010 INCITE award. Proposals for INCITE are due July 1, 2009.

Energy Sciences Network

Excellence.gov Honors ESnet

DOE's Energy Sciences Network (ESnet), a high-speed network linking tens of thousands of researchers around the nation, was honored April 14 with an Excellence.gov award for its excellence in leveraging technology. The awards are sponsored by the Industry Advisory Council's (IAC) Collaboration and Transformation Shared Interest Group and recognize the federal government's best information technology (IT) projects.

A panel of 25 judges—federal government and industry executives—reviewed the nominations and selected ESnet as the winner in the area of "Excellence in Leveraging Technology," one of five award categories. The winners were recognized at a ceremony in Washington, DC.

ESnet was honored for ESnet4, a recently completed network infrastructure providing highly-reliable, high-bandwidth connectivity to support and advance the United States' scientific competitiveness and capabilities by linking scientists at national laboratories and universities across the country. ESnet is funded primarily by the Office of Science and managed by Lawrence Berkeley National Laboratory.

Society for Industrial and Applied Mathematics

DOE Researchers Named as Fellows of SIAM

The Society for Industrial and Applied Mathematics (SIAM) announced its first class of Fellows on Friday, May 1, and the group included 13 current and retired mathematicians from DOE national laboratories. The society named 183 Fellows from its international membership of more than 12,000 mathematicians.

Of the DOE-affiliated fellows, five are from Lawrence Berkeley National Laboratory, four are from Los Alamos National Laboratory, two from Argonne National Laboratory and one from Oak Ridge National Laboratory. Additionally, two members of ASCR's Advisory Committee, ASCAC, were among the Fellows named.

"The announcement of the first class of SIAM Fellows is an important milestone for the applied mathematics and computational science community," said SIAM President Douglas N. Arnold. "Reflecting the diversity of the SIAM membership, these men and women come from five continents, and work in academia, industry, and government laboratories. Advancing the frontiers of research in branches of mathematics as distinct as number theory and partial differential equations, these professionals have applied their work to endeavors ranging from mining to medicine. They have designed algorithms to make computing possible and written textbooks to train the next generation of mathematicians. Their contributions are truly outstanding."

The DOE SIAM Fellows are:

Argonne National Laboratory

- Hans Kaper (retired), for contributions to differential equations and dynamics
- Jorge Moré, for advances in algorithms and software for continuous optimization

Brookhaven National Laboratory

- James Glimm (joint appointment at State University of New York at Stony Brook), for contributions to operator algebras, partial differential equations, mathematical physics, and especially shock wave theory

Lawrence Berkeley National Laboratory

- John Bell, for contributions to numerical methods for the partial differential equations of computational science
- Alexandre Chorin (joint appointment at University of California (UC)–Berkeley), for contributions to computational fluid dynamics
- Phillip Colella, for contributions to adaptive and numerical methods for partial differential equations in science and engineering
- James Demmell (joint appointment at UC–Berkeley), for contributions to numerical linear algebra, including the LAPACK project
- James Sethian (joint appointment at

UC–Berkeley), for contributions to the numerical solution of partial differential equations, especially level set methods

Los Alamos National Laboratory

- James "Mac" Hyman, for contributions to the numerical solution of partial differential equations and modeling of biological systems
- Alan Perelson, for contributions to viral dynamics and other problems of mathematical biology
- David Sharp, for contributions to dynamics and biology
- Burton Wendroff (retired), for contributions to the numerical solution of partial differential equations

Oak Ridge National Laboratory

- Jack Dongarra (joint appointment at University of Tennessee), for contributions to numerical linear algebra, including EISPACK, LINPACK, and LAPACK, and high-performance computing

Advanced Scientific Computing Advisory Committee (ASCAC)

- Marsha Berger, Courant Institute, New York University
- Thomas Manteuffel, University of Colorado–Boulder

Awards & Honors

Mark Seager Honored by *FCW*

Mark Seager (figure 2), Lawrence Livermore National Laboratory assistant department head for Advanced Technologies, has been selected by *Federal Computer Week* magazine as one of this year's "Federal 100" top executives from government, industry, and academia who had the greatest impact on government information systems in 2008.

Seager was selected because of "the difference [he] made in the way agencies, companies and government officials develop, acquire, manage and use information technology." The nomination was submitted by industry collaborators for Seager's leadership of the Hyperion Project, a collaboration with 10 industry leaders to advance next-generation Linux high-performance computing clusters.

"Hyperion represents a new way of doing business. Collectively we are building a system none of us could have built individually," Seager said when the project was announced at SC08 last November.



Figure 2. Mark Seager.

Keynote Speaker

Al Gore at SC09

SC09, the 22nd annual event in the SC conference series, recognized globally as the premier international conference on high-performance computing, networking, storage, and analysis, announced April 27 that it has selected former U.S. Vice President Al Gore to deliver the conference keynote address.

SC09 has adopted the theme of "Computing for a Changing World," and will present a special focus on initiatives related to Sustainability, Bio-Computing, and the 3D Internet.

"Al Gore has been a champion of applied computing technology for more than two decades," said Dr. Wilfred Pinfold, General Chair of SC09. "We are honored to name Al Gore as our SC09 keynote speaker."

Gore will deliver the keynote presentation on Thursday, November 19 for the anticipated crowd of 11,000 attendees made up of leading computational scientists, researchers, and super-computing experts from around the globe.



Figure 3. Karen Pao.



Figure 4. Lucy Nowell.

Advanced Scientific Computing Research

ASCR Welcomes Two New Program Managers

Karen Pao and Lucy Nowell have recently joined the Advanced Scientific Computing Research (ASCR) contingent of Program Managers.

Karen Pao (figure 3) is Program Manager for ASCR's applied math base programs. Karen says, "This is sort of a homecoming for me, as my training is in numerical analysis, and I did research in computational fluid dynamics before the twisted ways of fate brought me to DOE/NNSA HQ." Her biggest surprise at ASCR is the partition of "Base" and "SciDAC". She adds, "To me the boundary is never well-defined, can never be well-defined, and shouldn't be well-defined."

Karen Pao worked at the Los Alamos National Laboratory (LANL) for nearly 20 years. Karen's career at LANL has been a series of brushes with greatness, including an early-career exposure to high-performance computing and benchmarking, experimentation with C++ array class libraries, designing numerical schemes for slightly compressible flows, and, most recently, performing simulations and analyses of underground nuclear test output in the Hallowed Halls of the famous Top-Secret X-Division. She was on assignment with the fabled Advanced Simulation and Computing (ASC) Program at the Department of Energy/National Nuclear Security Administration Headquarters (DOE/NNSA HQ), where her primary assignment was to devise the ASC National Verification & Validation Strategy, when she

decided to stay in Washington, DC for good. Karen received her Ph.D. in Mathematics from UCLA in 1993.

Lucy Nowell (figure 4) will focus on ASCR's Data and Visualization programs. She comes to ASCR after an IPA assignment from Pacific Northwest National Laboratory (PNNL) to the National Science Foundation (NSF), where she was program director of the Office of Cyber-Infrastructure, in charge of the portfolio on data, data analysis, and visualization. Although the work is similar, she sees a big difference between the two agencies: "DOE is a mission agency, while NSF is very proudly not mission-driven, and supports a great deal of curiosity-driven research. NSF feels very much like an academic community and people there sometimes forget they are part of a federal agency, which is clearly not the case here."

Before going to NSF, Lucy was a Program Manager with the Advanced Research and Development Activity (ARDA), where she managed the programs on Novel Intelligence from Massive Data (NIMD), Geospatial Intelligence Information Visualization (GI2Vis), and Advanced Research in Interactive Visualization for Analysis (ARIVA). At PNNL, Lucy worked with the team that designed and developed the award-winning OmniViz bioinformatics software and contributed to patented user interface designs for ThemeRiverTM and AniViz (animated visualization).

Awards & Honors

Cecilia Aragon Named 2009 Woman of Vision

Hispanic Business magazine has honored Cecilia Aragon as one of 25 Women of Vision in 2009. As a staff scientist in the Computational Research Division at the DOE's Lawrence Berkeley National Laboratory, Aragon researches and develops collaborative visual interfaces to foster scientific insight. She is also a founding member of Latinas in Computing and is active in diversity and outreach programs at the Lab.

Before coming to the Lab in 2005, Aragon was a computer scientist at the NASA Ames Research Center and CEO of Top Flight Aviation, where she was an air show pilot, test pilot, and aerobatic champion. She received a Ph.D. in computer science from the University of California–Berkeley, and a Bachelor of Science degree in mathematics from the California Institute of Technology. She has authored or co-authored 30 peer-reviewed publications and over 100 other publications in computer science and astrophysics.

Awards & Honors

Timothy Scheibe Chosen as Darcy Lecturer

Each year an outstanding groundwater professional is chosen by a panel of scientists and engineers as the National Ground Water Research and Education Foundation's (NGWREF) Darcy Lecturer to share his or her work with their peers and students at universities both domestically and internationally. The 2010 honoree, the 24th overall and the first from a DOE Laboratory, is Dr. Timothy Scheibe, a staff scientist in the Hydrology Technical Group at Pacific Northwest National Laboratory. Dr. Scheibe has made major contributions to the field of groundwater modeling. His multidisciplinary and integrative approaches to computational modeling have brought new insights into the scaling of geochemical processes affecting contaminant transport and innovative methods to couple genome-based mechanistic understanding of biological processes with traditional groundwater modeling codes.