

Awards & Honors

Two SciDAC PIs Named 2009 ACM Fellows

Association for Computing Machinery (ACM) Fellows are recognized for their achievements in computing and computer science that have contributed fundamental knowledge to the field and generated a broad range of innovations in industry, commerce, entertainment, and education. Two SciDAC researchers (figure 1) are among the group of new Fellows announced for 2009.

Alok Choudhary of Northwestern University has been named a Fellow by the ACM “for contributions to High-Performance Computing, storage, and parallel I/O.” Dr. Choudhary is co-principal investigator of the SciDAC Scientific Data Management center.

Ian Foster, of Argonne National Laboratory and the University of Chicago, was named an ACM Fellow “for work in parallel programming languages, collaborative and distributed computing.” Dr. Foster is principal investigator on the SciDAC Center for Enabling Distributed Petascale Science project.



Figure 1. Recently named ACM Fellows, Dr. Ian Foster (left) and Dr. Alok Choudhary (right).

High-Performance Computing

ASCR-Funded Jaguar Heads the Top500

The Oak Ridge Leadership Computing Facility (OLCF) Cray XT5, known as Jaguar (figure 2), is the new number 1 supercomputer on the Top500 list. An upgrade from quad-core to six-core Opteron processors from Advanced Micro Devices (AMD) boosted Jaguar’s HPL performance to 1.76 petaflop/s. Jaguar, now with nearly a quarter of a million CPU cores, has a theoretical peak capability of 2.3 petaflop/s. The Linpack benchmark is used in determining the rankings of the Top500 list compiled by researchers at the University of Mannheim in Germany, the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (LBNL), and the University of Tennessee–Knoxville.

Other DOE systems in the top 20 include:

- Number 2, Roadrunner, the IBM system at Los Alamos, 1.042 petaflop/s
- Number 7, BlueGene/L at Lawrence Livermore, 478 teraflop/s
- Number 8, BlueGene/P at Argonne, 459 teraflop/s
- Number 10, Red Sky at Sandia, 424 teraflop/s
- Number 11, Dawn, a BlueGene/P system at Lawrence Livermore, 416 teraflop/s
- Number 15, Franklin, a Cray XT4 at NERSC, 266 teraflop/s
- Number 16, the Jaguar Cray XT4 system at Oak Ridge, 205 teraflop/s
- Number 17, Red Storm, a Cray XT3–XT4 system at Sandia, 204 teraflop/s

Further Information

<http://top500.org/lists/2009/11/press-release>



Figure 2. Jaguar’s Cray XT5 system ranks number 1 on the Top500 list. The XT4 system at Oak Ridge also made the top 20, coming in at number 16.

VACET, ESG Partner for Climate Tools that Offer New Insight into IPCC Data

The SciDAC Visualization and Analytic Center for Enabling Technologies (VACET) is working to help bring advanced visualization technology to the climate modeling and analysis community through a partnership with the Earth Systems Grid (ESG).

VACET worked closely with ESG during the second half of 2009 to prepare new tools, technologies, and material for presentation at the December 2009 climate meeting in Copenhagen.

Prior to working with VACET, the ESG visualization/analysis tool Climate Data Analysis Toolkit (CDAT) consisted of only one- and two-dimensional charting/plotting tools. VACET's role has been to roll out new three- and four-

dimensional visualization technologies that are now included in the CDAT release. This effort is beginning to bear fruit, with the first set of objectives: 3D slicing, isocontouring, multiple linked 3D views, and 3D moviemaking.

One image, a frame from the complete video which was shown in the WCRP booth at the climate meeting in Copenhagen, demonstrates the use of the visualization to communicate an important insight. The insight from this example is that the outer layer of the atmosphere is cooling while the lower layer is warming.

The other activity conducted in the process of developing the video was demonstrating

that the visualization could be realized in real time while transferring massive amounts of data. The real-time visualization demonstration was a finalist in the Supercomputing 2009 Bandwidth Challenge, held in November 2009. The team was recognized for demonstrating the transfer of 10 TB of climate data and producing the visualization in real time on the receiving end.

Further Information

VACET

<http://www.scidac.gov/viz/VACET.html>

ESG

<http://www.scidac.gov/compsci/ESG.html>

Awards & Honors

ASCR-Funded Computers Take Top Medals at SC09 HPC Challenge

The Oak Ridge Leadership Computing Facility (OLCF) Cray XT5 "Jaguar" took three gold medals and a bronze at the SC09 HPC Challenge. The IBM Blue Gene systems at Lawrence Livermore National Laboratory (LLNL) and Argonne Leadership Computing Facility (ALCF) won a gold, a silver, and a bronze.

Jaguar won first place for speed in solving a dense matrix of linear algebra equations by running the HPL software code at 1,533 trillion floating point operations per second (teraflop/s). Kraken, the world's fastest academic computer, took second by running HPL at 736 teraflop/s.

Jaguar also ranked first for sustainable memory bandwidth by running the STREAM code at 398 terabytes per second. STREAM measures how fast a node can fetch and store information.

Jaguar's third gold was for executing the Fast Fourier Transformation (FFT), a common algorithm used in many scientific applications, at 11 teraflop/s. Kraken took second with a speed of 8 teraflop/s.

Edged out by IBM Blue Gene machines at Lawrence Livermore and Argonne national laboratories, Jaguar took third place for run-



Figure 3. The annual SC is the international conference for high-performance computing, networking, storage, and analysis.

ning the RandomAccess measure of the rate of integer updates to random locations in a large global memory array.

The Blue Gene/L machine at LLNL took third in HPL and second in STREAM competitions, and the Japan Agency for Marine-Earth Science and Technology placed third in both STREAM and FFT contests.

High-Performance Computing

Magellan at SC09

A kickoff meeting for the Recovery Act-funded Magellan (cloud computing testbed) project was held at SC09. NERSC is inviting users to submit expressions of interest for the testbed, which will be available in early 2010.

The Magellan hardware will consist of 1,440 Intel Nehalem quad-core processors (5,760 cores total). Planned investigations include: comparative performance of scientific applications in cloud computing and traditional cluster/supercomputing environments; use of flash storage for data intensive applications; applications that can be ported to cloud computing models such as Hadoop (MAP/Reduce); creation of "science gateways" that use cloud computing to provide easy access to applications, databases, or automated workflows; alternative models for access to computing resources, such as use of virtual private clusters; and other novel and interesting proposals to apply cloud computing to enhance scientific research, or develop cloud computing software.

Further Information

<http://www.nersc.gov/nusers/accounts/magellan.php>

A New DOE ASCR SciDAC Initiative: ISICLES

The DOE Office of Advanced Scientific Computing Research (ASCR) recently funded six projects in response to the national and international need for better inclusion of dynamic ice sheet modeling in Earth System and Climate models. Collectively grouped as ISICLES (Ice Sheet Initiative for CLimate ExtremeS), this ASCR SciDAC Initiative is intended to accelerate computational science research for state-of-the-science algorithms and codes for ice sheet models that are scalable at extreme scales of computing.

A kickoff workshop for the ice sheet projects was held September 16–17, 2009, in Annapolis, Maryland. The goal was to coordinate the projects into a collective initiative to maximize their success and impact. The workshop opened with “View from the Office of the Under-Secretary for Science, Department of Energy” presented by Dr. David Dean, Senior Advisor, Office of the Under-Secretary for Science, DOE. This was followed by “Perspectives from the Office of Advanced Scientific Computing Research (OASCR), DOE” presented by Dr. Walt Polansky, Division Director for Research, OASCR.

Organized by the DOE ASCR Program Manager, Dr. Lali Chatterjee, the workshop included presentations from Dr. Robert Bindschadler, Chief Scientist, NASA Goddard Space Flight Center, and Dr. Tony Payne, University of Bristol, United Kingdom. These addressed the critical importance of computational science advances on ice sheet dynamics and their inclusion in climate models. Dr. David Keyes, University of Columbia, talked about key mathematical techniques and software issues, and Dr. Jim Hack, Director, National Center for Computational Sciences at Oak Ridge National Laboratory (ORNL), discussed the regional impacts of ice sheet melting. Dr. W. Lipscomb, Los Alamos National Laboratory (LANL) presented on the existing models, and each project highlighted its objectives. DOE Program Managers – Dr. Chatterjee (ASCR) and Dr. A. Bamzai (BER) – led the discussions on future projections, milestones, and expectations.

This ISICLES initiative also represents an expansion of ASCR’s existing Computational Partnerships with the Office of Biological and Environmental Research (OBER), for DOE SC Climate Modeling efforts as computationally strong and robust ice sheet and climate codes are naturally, and critically, dependent on the correct science input. The projects are led by four national labs (Argonne, Lawrence Berke-



Figure 4. The Ice Sheet Initiative for Climate ExtremeS (ISICLES) is a set of ASCR/SciDAC projects intended to accelerate computational science research for state-of-the-science algorithms and codes for ice sheet models that are scalable at extreme scales of computing.

ley, Oak Ridge, and Pacific Northwest) and two universities (Columbia and the University of Texas); LANL is collaborating with five projects, and Sandia National Laboratories with two. Planned investigations include:

- Working within SEA-CISM, a project led by ORNL (Kate Evans, principal investigator) will implement the Trilinos framework around a hierarchical blocking structure for increased parallelism, using implicit solver capabilities and physics-based preconditioning to maximize scalability
- B-ISICLES, an effort led at Berkeley Lab (Esmond Ng, principal investigator) will leverage expertise in block-structured adaptive mesh refinement to develop a parallel and scalable Community Ice Sheet Model (CISM) in the Chombo solver framework
- SISIPHUS (Scalable Ice Sheet Solvers and Infrastructure for Petascale) is a project led at Argonne (Tim Tautges, principal investigator) will develop techniques for solving the full three-dimensional Stokes problem using hp-adaptive finite element methods, with the PETSc solvers as a base and careful consideration of the interfaces to allow forward and adjoint solutions
- A group based at the University of Texas (Omar Ghattas, principal investigator) is developing a full-Stokes flow model with adaptive grid

refinement, high-order discretizations, forward and inverse problem solving capability, and scalable uncertainty quantification techniques

- Using extended finite elements to capture discontinuities with “self-correcting” and algebraic multigrid methods, a project led by Columbia University (Haim Waisman, principal investigator) will develop scalable models of the complex fracture of ice within larger ice sheet models
- A project led by Pacific Northwest Laboratory (Alexander Tartakovsky, principal investigator) will develop a three-dimensional Lagrangian particle ice sheet model based on the fundamental conservation equations, using algorithms based on smooth particle hydrodynamics to achieve scalability

Since inclusion of “fully dynamic ice sheet models and ocean/ice shelf interactions,” prioritized by the “Joint ASCAC-BERAC Report” in March 2008, are still in their early stages of development, ISICLES has the potential to make a notable difference. Incorporation of advanced techniques of high-performance and extreme scale computing in the early stages of code creation will better ensure their effective use, rather than introduction of these techniques into established codes. ISICLES is not only expected to have a strong impact on DOE’s climate models and codes, but also planned to extend to other national and international models.