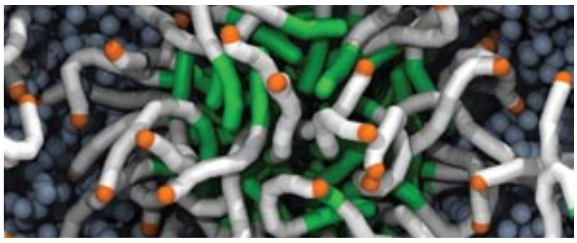
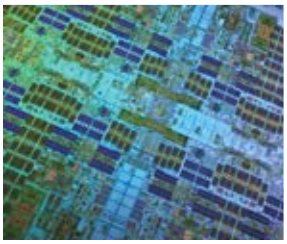
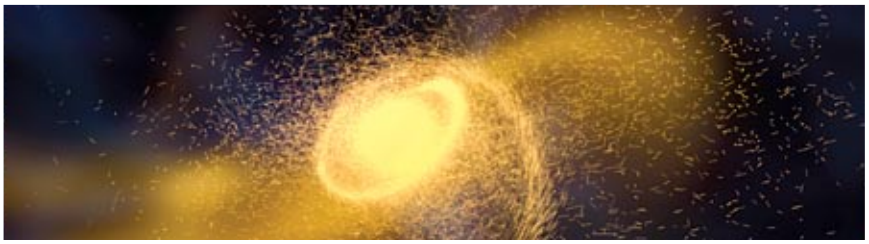
BLUE WATERS PROJECT
QUARTERLY NEWSLETTER







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IBM Provides Details on Blue Waters

THE GOAL of the Blue Waters Project is to provide a robust, reliable petascale computing system that can solve the most challenging compute-, data- and memory intensive problems in science and engineering. At Hot Chips 2009 and SC09 IBM provided new details on the POWER7 chip as well as the Blue Waters sustained petascale computing system. This information illustrates how Blue Waters will achieve these goals.

POWER7 CHIP: IBM's new POWER7 chip, which is the heart of Blue Waters, will have:

- 8 cores
- Simultaneous multithreading with up to 4 threads per core
- 3 levels of on-chip cache (L1: 64 KB (I), 64 KB (D); L2: 256 KB; L3: 32 MB)
- 128 GB/s peak memory bandwidth
- Up to 256 GFLOPS peak performance (depending on frequency); 8 FLOPS per cycle
- Frequency from 3.5 to 4.0 GHz

The L1 and L2 caches are fast SRAM, while the large L3 cache is dense, slower but low power eDRAM. The L3 cache has both private and shared spaces that can be reconfigured on the fly to provide better efficiency for multithreaded programs and to support efficient prefetching.

BLUE WATERS SYSTEM: At SC09 IBM revealed that the Blue Waters System will be built on quad-chip modules (QCMs) with each module having:

- Four (4) POWER7 chips,
- 128 GB of memory
- 512 GB/s memory peak bandwidth
- Up to 1 TFLOPS peak performance
- 192 GB/s messaging and I/O bandwidth off the QCM

Eight QCMs will be configured in a compute "drawer," along with eight Hub chips and associated cabling, 1 TB of memory, and power supplies (see Figure 1). The Hub chip can handle over 1.1 TB/s: 192 GB/s to the host QCM, 336 GB/s to the seven other Hub chips in the drawer, 240 GB/s to Hub chips for three other local-drawers, 320 GB/s to remote drawers, and a 40 GB/s general purpose I/O.

All of the hardware in the drawer – QCMs, memory, Hub chips – are directly water cooled. This increases the efficiency of both the computer and the cooling system. Because the components are directly water-cooled, no air has to be moved around; because the electronics run cooler, they dissipate less power.

Additional information on the POWER7 chip and the Blue Waters System will be posted on the Blue Waters website:
www.ncsa.uiuc.edu/BlueWaters/hardware.html

A Blue Waters compute drawer on display in the IBM booth at SC09.

Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign, its National Center for Supercomputing Applications, IBM, and the Great Lakes Consortium for Petascale Computation. It is supported by the National Science Foundation, the University of Illinois at Urbana-Champaign, and the state of Illinois.

Research Teams Win PRAC Awards

EIGHTEEN RESEARCH TEAMS involving scientists and engineers from 30 institutions recently received Petascale Computing Resource Allocations (PRAC) from NSF. PRAC awards provide allocations or provisional allocations of computing time on Blue Waters as well as travel funds to enable the approved research teams to work closely with the Blue Waters Project Team at NCSA to tune and optimize their science and engineering applications to take full advantage of the capabilities of Blue Waters. The projects that received PRAC awards are listed below.

The Computational Microscope, Klaus Schulten and Laxmikant Kale, University of Illinois at Urbana-Champaign

Petascale Simulations of Complex Biological Behavior in Fluctuating Environments, Ilias Tagkopoulos, University of California, Davis

Petascale Computations for Complex Turbulent Flows, Pui-Kuen Yeung, James Riley, and Amitava Majumdar, Georgia Institute of Technology; Robert Moser, Universtiy of Texas Austin

Petascale Research in Earthquake System Science on Blue Waters, Thomas Jordan and Jacobo Bielak, University of Southern California

Enabling Large-Scale, High-Resolution and Real-Time Earthquake Simulations on Petascale Parallel Computers, Liqiang Wang and Po Chen, University of Wyoming

Testing Hypotheses about Climate Prediction at Unprecedented Resolutions on Blue Waters, David Randall and Ross Heikes, Colorado State University; William Large, Richard Loft, John Dennis and Mariana Vertenstein, University Corporation for Atmospheric Research; Cristiana Stan and James Kinter, Institute of Global Environment and Society; Benjamin Kirtman, University of Miami

Understanding Tornados and Their Parent Supercells through High Resolution Simulations and Analysis, Robert Wilhelmson and Brian Jewett, University of Illinois at Urbana-Champaign and Mathew Gilmore, University of North Dakota

Computational Relativity and Gravitation at the Petascale: Simulating and Visualizing Astrophysically Realistic Compact Binaries, Manuela Campanelli, Carlos Lousto, Hans-Peter Bischof, Joshua Faber, Yosef Ziochower, Rochester Institute of Technology

Enabling Science at the Petascale: From Binary Systems and Stellar Core Collapse to Gamma-Ray Bursts, Eric Schnetter, Gabrielle Allen, Mayank Tyagi, Peter Diener, and Christian Ott, Louisiana State University

Formation of the First Galaxies: Predictions for the Next Generation of Observatories, Brian O'Shea, Michigan State University and Michael Norman, University of California, San Diego

Peta-Cosmology: Galaxy Formation and Virtual astronomy, Kentaro Nagamine, University of Nevada, Las Vegas; Jeremiah Ostriker and Renyue Cen, Princeton University; Greg Bryan, Columbia University

Petascale Simulation of Turbulent Stellar Hydrodynamics, Paul Woodward, and Pen-Chung Yew, University of Minnesota

Computational Chemistry at the Petascale, Monica Lamm, Mark Gordon, Theresa Windus, and Masha Sosonkina, Iowa State University; Brett Bode, University of Illinois at Urbana-Champaign

Super Instruction Architecture for Petascale Computing, Rodney Bartllet, Erik Duemens and Beverly Sanders, University of Florida and Ponnuswamy Sadayappan, The Ohio State University

Breakthrough Petascale Quantum Monte Carlo Calculations, Shiwei Zhang, College of William and Mary

Electronic Properties of Strongly Correlated Systems Using Petascale Computing, Sergey Savrasov, University of California, Davis; Kristjan Haule and Gabriel Kotliar, Rutgers University

Lattice QCD on Blue Waters, Robert Sugar, University of California, Santa Barbara

Simulation of Contagion on Very Large Social Networks with Blue Waters, Keith Bisset and Xizhou Feng, Virginia Polytechnic Institute and State University; Shawn Brown, Carnegie-Mellon University; Douglas Roberts, Research Triangle University

Additional information on the PRAC awards, and a link to the NSF solicitation, can be found at:

www.ncsa.illinois.edu/BlueWaters/prac.html

Computing Resource Allocations on Blue Waters (PRAC)

Proposals for the next PRAC competition are due to NSF on March 17, 2010. Allocations on Blue Waters can only be obtained through the PRAC process, so researchers who desire early access to Blue Waters must apply now.

Dan Katz at the University of Chicago's Computation Institute is available to pro¬vide guidance to research teams interested in submitting a PRAC proposal to NSF. He can be contacted at dsk@uchicago.edu.

On Feb. 1, NCSA hosted a two-hour webinar to provide details about the Blue Waters system, an overview of the PRAC program, and tips on writing successful PRAC proposals. Presenters include Katz and the Blue Waters staff. The PowerPoint from the presentation as well as other PRAC information can be found on the PRAC website: www.ncsa.illinois.edu/BlueWaters/prac.html.

Collaborative Software Development Projects

THE COMPUTING SYSTEM SOFTWARE is an equally critical part of the Blue Waters Petascale Computing System. A major effort in the Blue Waters Project is focused on enhancing IBM's high-performance computing environment to ensure that applications achieve high sustained performance. This environment will also enhance the productivity of application developers and system administrators by providing a convenient, integrated set of tools to analyze and control the behavior of the system. Major collaborative projects underway with IBM include:

- **PETASCALE APPLICATION DEVELOPMENT ENVIRONMENT**
  A PADE is being developed to support application development at the petascale. The PADE will support all of the major scientific computing languages, including UPC and CAF and will provide syntax aware editors and interfaces to compilers, tuning and debugging tools, job submission and control tools, and workflow engines. The client environment is based on the open source Eclipse platform.
- **COMPUTATIONAL LIBRARIES**
  A number of the libraries needed by the PRAC awardees are being ported and tuned for Blue Waters. In addition to IBM's ESSL and PESSL libraries, these include PETSc, SPRNG and pnetCDF.
- **INTEGRATED SYSTEM CONSOLE**

  IBM and NCSA are developing a comprehensive system management environment to provide the integration necessary to support a system of the scale of Blue Waters. The ISC will coordinate system monitoring, checkpointing, RAID-recovery, and interconnect reconfiguration and will present a unified, command/observation visual interface to the system administration team.

- **PERFORMANCE MODELING**

  NCSA is working, in collaboration with the team of Adolfy Hoisie and Darren Kerbyson at LANL and the team of Alan Snavely at UCSD, to improve performance-modeling capabilities for Blue Waters. The goal is to develop a more systematic performance engineering methodology that will ensure codes get the best possible performance on Blue Waters, and are ready to run as soon as the system is available. A workshop is coming in March, check the Blue Waters website for information.

Virtual School of Computational Science & Engineering

PREPARATION FOR PETASCALE COMPUTING requires solid grounding in computational science and engineering and scientific computing, especially on HPC and HPC-related issues. To help address this problem, the Blue Waters Project is providing seed funding for the Virtual School of Computational Science and Engineering (VSCSE) that brings together faculty from throughout the country to create courses that focus on petascale computing and petascale-enabled science and engineering.
Summer schools

The VSCSE held one class in 2008 and two summer school courses in 2009. Many-Core Processors and Scaling to Petascale were each hosted simultaneously by four institutions (including LSU, ORNL, NCSA, OSU, UIC, and UM) via a high-definition video link. Total attendance for the two schools was 232 students.

This summer, course offerings as well as the number of host sites and participating students will increase. If your site is interested in participating in Summer School 2010, just follow the directions found at:

http://bit.ly/2iedUR

Great Lakes Consortium for Petascale Computation

THE GOAL OF THE GLCPC is to facilitate and coordinate multi-institutional efforts to advance computational science and engineering, technology research, education and their applications to problems of regional or national importance. Twenty-eight institutions are consortium members.

One effort to achieve the goal has been a series of scheduled presentations on the campuses of GLCPC member universities. These presentations introduce petascale computing and the Blue Waters Project to interested faculty, students, and researchers. GLCPC member organizations should contact Anita Broeren of NCSA (abroeren@ncsa.uiuc.edu) to schedule a presentation on their campus.

The GLCPC has committees established to address both the software and hardware infrastructure of Blue Waters, along with committees for new membership, system allocation and industry involvement. In addition, an executive committee was established in 2009: President, John Ziebarth, Krell Institute; Maxine Brown, University of Illinois-Chicago; William Punch, Michigan State University; Stan Ahalt, RENCI/University of North Carolina; Srinivas Aluru, Iowa State University; Padma Raghavan, Pennsylvania State University; and Tom Jones, University of Minnesota. Committee chairs and other GLCPC information can be found on the GLCPC website:

www.greatlakesconsortium.org

Petascale Computing Facility Nears Completion

THE NEW STATE-OF-THE-ART 88,000-square-foot National Petascale Computing Facility (NPCF) is finishing construction on the University of Illinois' south campus to house Blue Waters and other NCSA computing infrastructure, as well as nearly 40 staff members. The facility includes a 20,000-square-foot data center with an additional 10,000 square feet of raised floor for other infrastructure. It will be large enough to simultaneously accommodate the Blue Waters system, a follow-on system, and

several smaller systems. It combines top-flight physical and cybersecurity with the open, collaborative research attitude of a public educational institution.

Energy efficiency is an integral part of the Blue Waters Project and the NPCF. The facility will:

- Achieve LEED Silver certification, with LEED Gold as the goal.
- Take advantage of very efficient on-site cooling towers to chill water for all building and computer cooling needs. This reduces energy consumption by using outside air to chill water up to 70 percent of the year. The facility will also take advantage of the campus' highly reliable electricity supply, avoiding the need for the standard back-up Uninterruptible Power Supply (UPS).
- Run high-voltage AC power directly to the rack. The computer will the convert the 480 volt AC power to DC power thus avoiding power losses associated with power conversion, again saving energy.
- The Power Usage Efficiency (PUE) is estimated to be less than 1.2, with a PUE of less than 1.1 during much of the year. Current computing facilities have PUEs ranging from 1.4 to 2.0.

Substantial completion of the new facility will occur in March, well ahead of schedule, with the installation of computing equipment beginning in the summer. To view the facility or watch the construction webcam go to:

www.ncsa.illinois.edu/AboutUs/Facilities/pcf.html

Joint Laboratory for Petascale Computing

IN JUNE 2009 the Center for Extreme-scale Computation in the University of Illinois' Institute for Advanced Computing Applications & Technology signed an agreement with the French National Institute for Research in Computer Science and Control (INRIA) to establish a Joint Laboratory for Petascale Computing. The Joint Laboratory is focused on collaborative research aimed at realizing the full potential of petascale computing, in particular the Blue Waters sustained petascale computing system.

The Joint Laboratory held its second workshop at NCSA on December 2-4, 2009. Topics discussed at the workshop included: Blue Waters hardware and software, Algorithms and numerical libraries, Fault tolerance, New programming models, and Hybrid computing.

More than 40 scientists from Illinois and INRIA participated in the workshop, which identified additional collaborative projects in combining atom level and molecular level simulations (NAMD + Big DFT), fault-tolerance and resilence at petascale and beyond, runtime system solutions for heterogeneous programming (MPI+OpenMP+CUDA), dynamic remapping of distributed executions, MILC code memory optimization for QCD, communication avoiding numerical libraries, I/O system interface and scheduling. The next workshop will be June 2010 in Bordeaux, France. For more information on the Joint Laboratory, including the presentations given at the workshop, see:

jointlab.ncsa.illinois.edu

Events of Interest

- Writing successful PRAC proposals webinar, February 1, 2010
  www.ncsa.illinois.edu/News/10/0105Feb1webinar.html
- Application Performance Modeling Workshop, early March, TBD
  www.ncsa.illinois.edu/BlueWaters/
- Extreme-Scale I/O and Data Analysis, March 22-24, 2010, Austin, TX
  http://bit.ly/63Cx6z
- Scaling to Petascale, July 6-9, 2010, multiple locations
  www.vscse.org/summerschool/2010/workshops.html
- Big Data for Science July 26-30, 2010, multiple locations
  www.vscse.org/summerschool/2010/workshops.html
- 5th Annual TeraGrid Conference, August 2-5, 2010, Pittsburgh, PA
  www.teragrid.org
- Many-Core Processors, August 2-6, 2010 multiple locations
  www.vscse.org/summerschool/2010/workshops.html

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