Argonne NATIONAL LABORATORY

TRANSFORMING THE WORLD THROUGH BREAKTHROUGH SCIENCE

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Transforming the World through Breakthrough Science at the ALCF

The word "breakthrough" aptly describes the transformational science and milestones achieved at the Argonne Leadership Computing Facility (ALCF) throughout 2008.

The number of research endeavors undertaken at the ALCF through the U.S. Department of Energy's (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program grew from 9 in 2007 to 20 in 2008. The allocation of computer time awarded to researchers on the Blue Gene/P also spiked significantly—from nearly 10 million processor hours in 2007 to 111 million in 2008. To support this research, we expanded the capabilities of Intrepid, an IBM Blue Gene/P system at the ALCF, to 557 teraflops (TF) for production use. Furthermore, we enabled breakthrough levels of productivity and capability in visualization and data analysis with Eureka, a powerful installation of NVIDIA Quadro Plex S4 external graphics processing units. Eureka delivered a quantum leap in visual compute density, providing more than 111 TF and more than 3.2 terabytes of RAM.

On April 21, 2008, the dedication of the ALCF realized DOE's vision to bring the power of the Department's high performance computing to open scientific research. In June, the IBM Blue Gene/P supercomputer at the ALCF debuted as the world's fastest for open science and third fastest overall.

No question that the science benefited from this growth and system improvement. Four research projects spearheaded by Argonne National Laboratory computer scientists and ALCF users were named to the list of top ten scientific accomplishments supported by DOE's Advanced Scientific Computing Research (ASCR) program. Three of the top ten projects used extensive grants of computing time on the ALCF's Blue Gene/P to model the molecular basis of Parkinson's disease, design proteins at atomic scale, and create enzymes.

As the year came to a close, the ALCF was recognized with several prestigious awards at SC08 in November. We provided resources for Linear Scaling Divide-and-Conquer Electronic Structure Calculations for Thousand Atom Nanostructures, a collaborative effort between Argonne, Lawrence Berkeley National Laboratory, and Oak Ridge National Laboratory that received the ACM Gordon Bell Prize Special Award for Algorithmic Innovation. The ALCF also was named a winner in two of the four categories in the HPC Challenge best performance benchmark competition.

Future of Computational Science

In the future, we believe that several key issues and trends in high performance computing will impact the delivery of breakthrough science and engineering at the ALCF.

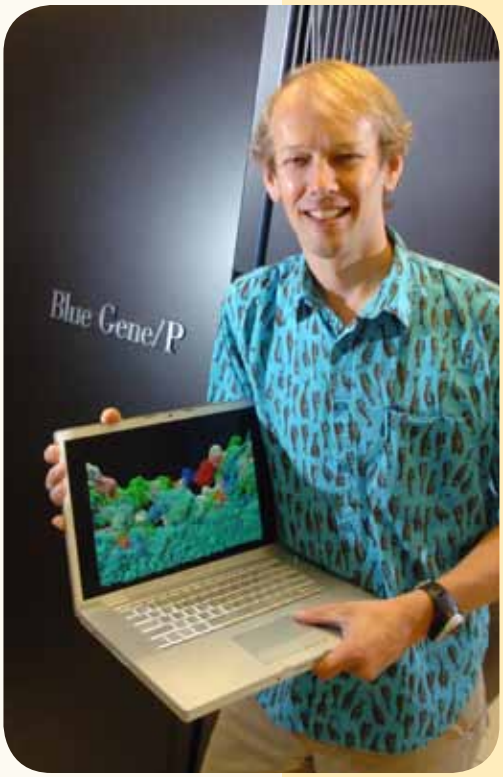
For instance, modeling and simulation are playing a greater role in all areas of scientific disciplines — from understanding the molecular processes in cells to designing next-generation batteries for hybrid vehicles. For many disciplines, computation is not only the fastest and most cost-effective tool for discovery, it is the *principal* one. For example, understanding the evolution of our galaxy, the future climate of the planet, or the spread of influenza through populations is difficult without supercomputing.

We're also working with the international community to improve the software supporting science on the next generation of extreme-scale platforms. The International Exascale Software Project has launched a series of workshops to explore how the community can better integrate and develop the open source software components that run the world's fastest computers. But the future of software is only half of the story. In partnership with Lawrence Livermore National Laboratory and IBM, we're designing the next-generation supercomputer platform, which will be many times more powerful, yet more power-efficient, than the current generation of systems.

Finally, while we have had great success with building a world-class computational facility, the ALCF can't deliver scientific discoveries without top computational scientists. Bringing these scientists on board is crucial to addressing scientific problems quickly and comprehensively. As a result, we rely on the nation's continuing investment in science and technology educational programs. They are instrumental to our success in recruiting and retaining the most highly-qualified computational scientists.

As we lay the foundation for the ALCF's progression to exascale computing, we will relocate to a new Theory and Computing Sciences building on Argonne's site in 2009. The 200,000-square-foot building will house all ALCF staff as well as that of the Mathematics and Computer Science Division, strengthening our already close collaborations. It has also been designed to accommodate our next-generation supercomputers. Through this state-of-the-art facility and key partnerships, we'll advance computer science and key application fields significantly, both now and in the future.

Dr. Peter Beckman
ALCF Director



About Argonne National Laboratory

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

Availability of This Report

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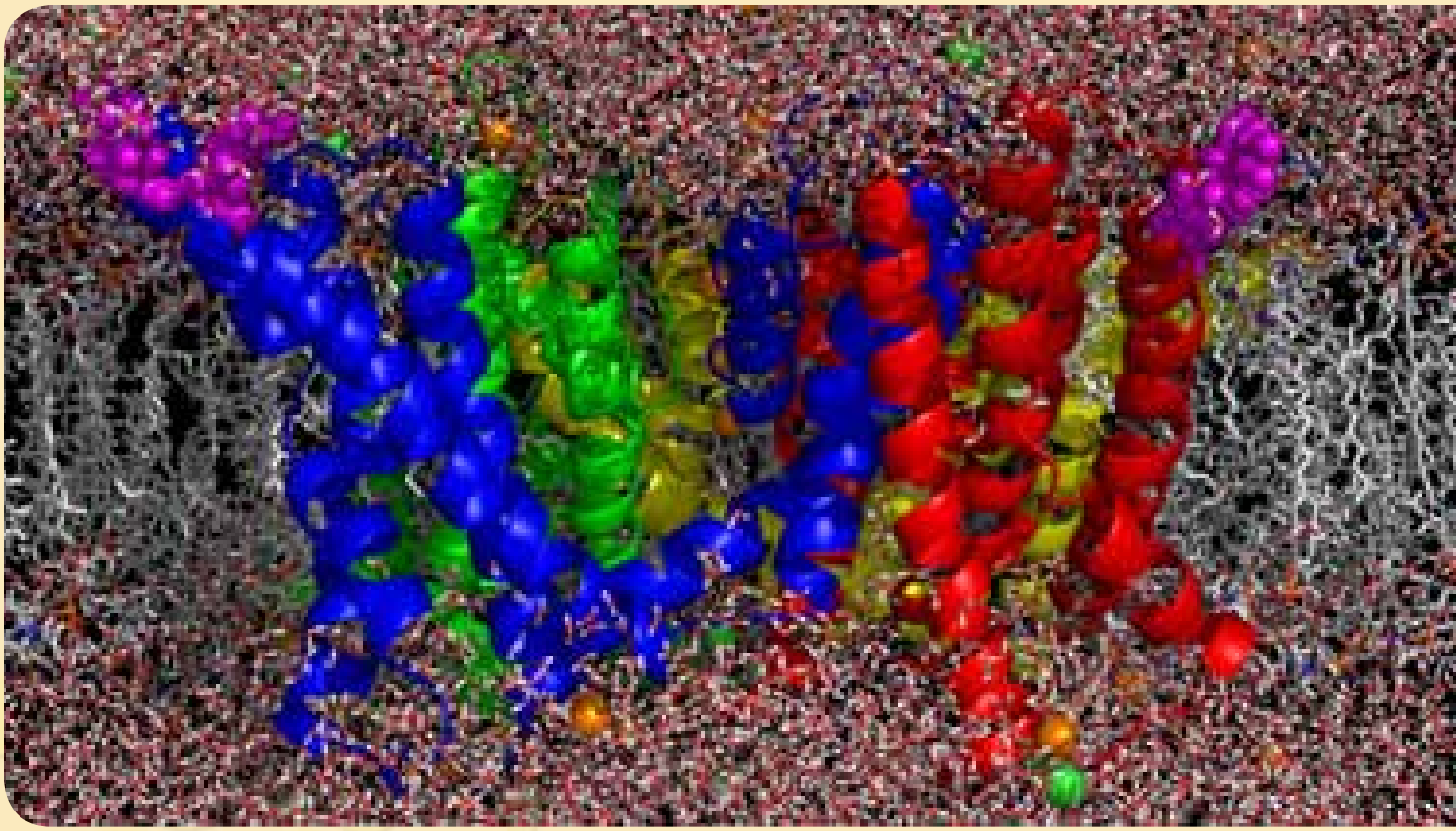
table of contents



ALCF OVERVIEW

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ALCF Provides Science Community with Leadership-Class Computing

Mission

The mission of the Argonne Leadership Computing Facility (ALCF) is to accelerate major scientific discoveries and engineering breakthroughs for humanity by designing and providing world-leading computing facilities in partnership with the computational science community. A U.S. Department of Energy (DOE) national leadership-class computing facility, the ALCF is sponsored by DOE's Office of Advanced Scientific Computing Research in the Office of Science.

Vision

The ALCF strives to be the forefront computational center for extending the frontiers of science by solving key problems for the nation that require innovative approaches and the largest-scale systems.

Research and Resources

DOE selects major research endeavors to be carried out on ALCF resources through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This program seeks large-scale, computationally intensive research projects that can make high-impact scientific advances through the use of a major allocation of computer time, resources, and data storage. (See next page for more details about the INCITE program.) In addition, a portion of the ALCF's projects are conducted through discretionary allocations.

Researchers who receive INCITE or discretionary allocations at the ALCF use the IBM Blue Gene/P system named Intrepid, one of the world's fastest supercomputers. The ALCF also operates Surveyor, a Blue Gene/P system used for tool and application porting, software testing and optimization, and systems software development, as well as Eureka, a visualization supercomputer that allows researchers to explore and visualize the flood of data they produce with Intrepid.

User Services

ALCF staff members provide users with in-depth expertise and assistance in using ALCF computer systems and achieving the best performance in their applications. The staff establishes strategic collaborations with the ALCF's project partners to maximize the benefits from using ALCF resources.

Sampling of ALCF Staff

2008 INCITE Projects at ALCF

Based on their potential for breakthroughs in science and engineering, DOE awarded 20 research projects more than 111 million hours of computing time at the Argonne Leadership Computing Facility (ALCF) in 2008. The awards were made through DOE's INCITE program.

The following INCITE projects represented a wide array of scientific disciplines, ranging from climate research to engineering physics and materials science to life sciences. (See 2008 Research Discoveries on pp. 11-22 for research achievements.)

- Climate-Science Computational End Station Development and Grand Challenge Team
- Computational Nuclear Structure
- Computational Protein Structure Prediction and Protein Design
- Gating Mechanism of Membrane Proteins
- High-Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability
- High-Resolution Global Simulation of Plasma Microturbulence
- Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles
- Large-Scale Simulations of Cardiac Electrical Activity
- Lattice QCD
- Massively Parallel Simulation of Combustion in Gas Turbines
- Modeling the Rheological Properties of Concrete
- Molecular Simulation of Complex Chemical Systems
- Molecular Simulation of Surfactant-Assisted Aqueous Foam Formations
- Performance Evaluation and Analysis Consortium End Station
- Plan 9 Measurements on Large-Scale Systems
- Predictions of Thermal Striping in Sodium-Cooled Reactors
- Reactor Core Hydrodynamics
- Simulation and Modeling of Synuclein-Based Protofibril Structures as a Means of Understanding the Molecular Basis of Parkinson's Disease
- Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernovae Models
- Water in Confined States

DOE INCITE Program

The U.S. Department of Energy's (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program annually awards researchers millions of supercomputer processor hours at DOE's global flagship facilities for unclassified supercomputing. These facilities, including the Argonne Leadership Computing Facility (ALCF), house some of the most powerful computers in the world.

The INCITE program encourages proposals from industry, universities, and research institutions. Proposals are peer-reviewed and chosen solely on the basis of scientific merit and readiness to use the LCF computers at scale. More information about the program can be found on DOE's Office of Science website at *http://science.doe.gov/ascr/INCITE/index.html*

Intrepid's Green System Delivers More "Science Per Watt"

The Argonne Leadership Computing Facility (ALCF) houses the powerful IBM Blue Gene/P supercomputer named Intrepid, which debuted in June 2008 as the world's fastest computer for open science and third fastest overall. Intrepid offers a peak speed of 557 teraflops (TF) and a LINPACK speed of 450 TF. It has 40,960 nodes, each with four processors or cores for a total of 163,840 cores and 80 terabytes of memory.

Intrepid's green system and supporting data center is managed efficiently from the ground up. Blue Gene/P features a low-power, system-on-a-chip architecture and communications fabric that enables science applications to scale efficiently to the highest performance with less electricity. By increasing the system's parallelism and using more power-efficient voltages and clock speeds, Intrepid permits scientists to explore the universe with computation with but a trickle of electricity compared to alternative architectures.

The Blue Gene/P uses about one-third as much electricity as a machine of comparable size built with more conventional parts. Of general-purpose, homogeneous architecture supercomputers, the Blue Gene/P is the most power efficient. Furthermore, by leveraging the Chicago area's cold winters to chill the cooling system water for free, the ALCF saves millions of dollars a year in electrical power compared to other similarly sized supercomputer centers.

The supercomputer's data systems consist of 640 I/O nodes that connect to 16 storage area networks (SANs) that control 7,680 disk drives with a total capacity of 7.6 petabytes of raw storage and a maximum aggregate transfer speed of 88 gigabytes per second. The ALCF uses two parallel file systems—PVFS and GPFS—to manage the storage. An HPSS automated tape storage system provides archival storage.

Blue Gene/P Resources

Intrepid

Production scientific and engineering computing

- 40,960 quad-core compute nodes
- 163,840 processors
- Memory: 80 terabytes
- Peak Performance: 557 teraflops

Surveyor

Tool and application porting, software testing and optimization, and systems software development

- 1,024 quad-core nodes
- 4,096 processors
- Memory: 2 terabytes
- Peak Performance: 13.9 teraflops

Eureka

Visualization and data analytics to transform data into useful knowledge.

- 100 dual quad-core servers
- 200 NVIDIA Quadro FX5600 GPUs
- Memory: More than 3.2 terabytes of RAM
- Peak Performance: More than 111 teraflops

ALCF also operates Surveyor, a Blue Gene/P system with 1,024 quad-core nodes (4,096 processors) and 2 terabytes of memory. Surveyor is used for tool application porting, software testing and optimization, and systems software development.

Data analytics and visualization are handled through one of the world's largest installations of NVIDIA Quadro Plex S4 external graphics processing units (GPU). Nicknamed Eureka, the visualization supercomputer is also very power efficient, and allows researchers to explore and visualize the torrents of data they produce with Intrepid at the ALCF. The installation provides more than 111 TF and more than 3.2 terabytes of RAM (5% of Intrepid's RAM).

The computational engine, the data storage, and the analytics system are all key components in the scientist's workflow. ALCF staff is continuing to improve both the software environment so that scientists can be more productive and the electrical efficiency so that users can achieve more "science per watt." These enhancements ensure that the ALCF is one of the most productive and power-efficient computational science centers in the world.

ALCF HIGHLIGHTS

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ALCF Dedicated in April

Argonne National Laboratory celebrated the dedication of the ALCF during an April 21, 2008 ceremony at the Lab.

"*I am delighted to see this realization of our vision to bring the power of the Department's high performance computing to open scientific research*," said DOE Under Secretary for Science Dr. Raymond L. Orbach. "*This facility will not only strengthen our scientific capability but also advance the competitiveness of the region and our nation.*" The early results span the gamut from determining the origins of the universe and dark energy, to better understanding the molecular mechanism of Parkinson's disease progression to help focus the search for treatment.

Dr. Patricia Dehmer, DOE Office of Science Deputy Director for Science Programs, and Dr. Michael Strayer, DOE Associate Director of Science for Advanced Scientific Computing Research, attended the ALCF dedication, along with Dr. Orbach and Congresswoman Judy Biggert.

Blue Gene/P Debuts as World's Fastest for Open Science, Third Overall

The IBM Blue Gene/P high performance computing system debuted as the fastest supercomputer in the world for open science, according to the semiannual TOP500 List of the world's fastest computers. The TOP500 List was announced on June 18, 2008 during the International Supercomputing Conference in Dresden, Germany.

The Blue Gene/P—known as Intrepid and located at the ALCF—also ranked third fastest overall. The Blue Gene/P has a peak-performance of 557 teraflops (557,056,000 million calculations per second). Intrepid achieved a speed of 450.3 teraflops on the LINPACK benchmark used to measure speed for the TOP500 rankings.

Four Argonne Projects Recognized among DOE's Top 10 Scientific Achievements

Four projects spearheaded by Argonne computer scientists and users of the ALCF have been named to the list of top ten scientific accomplishments supported by DOE's Advanced Scientific Computing Research (ASCR) program.

Three of the top ten ASCR projects are using extensive grants of computing time on the Blue Gene/P at the ALCF to conduct large-scale calculations needed to achieve new scientific discoveries. These projects are focusing on modeling the molecular basis of Parkinson's disease (lead: Igor Tsigelny, University of California-San Diego); designing proteins at atomic scale and creating enzymes (lead: David Baker, University of Washington); and exploring the mysteries of

water (lead: Giulia Galli, University of California-Davis). Another award-winning project, PETSc, a portable, extensible software toolkit, is being developed by researchers in Argonne's Mathematics and Computer Science Division (lead: Barry Smith) to support high-performance petascale and terascale simulations based on partial differential equations.

Beckman Named Director of Argonne's Leadership Computing Facility

Peter Beckman was named director of the Leadership Computing Facility Division at Argonne National Laboratory. The Leadership Computing Facility operates the ALCF, which is home to the Blue Gene/P and part of the U.S. Department of Energy's effort to provide leadership-class computing resources to the scientific community. Beckman also leads Argonne's exascale computing strategic initiative and has previously served as the ALCF's chief architect and project director. He has worked in systems software for parallel computing, operating systems, and Grid computing for 20 years.

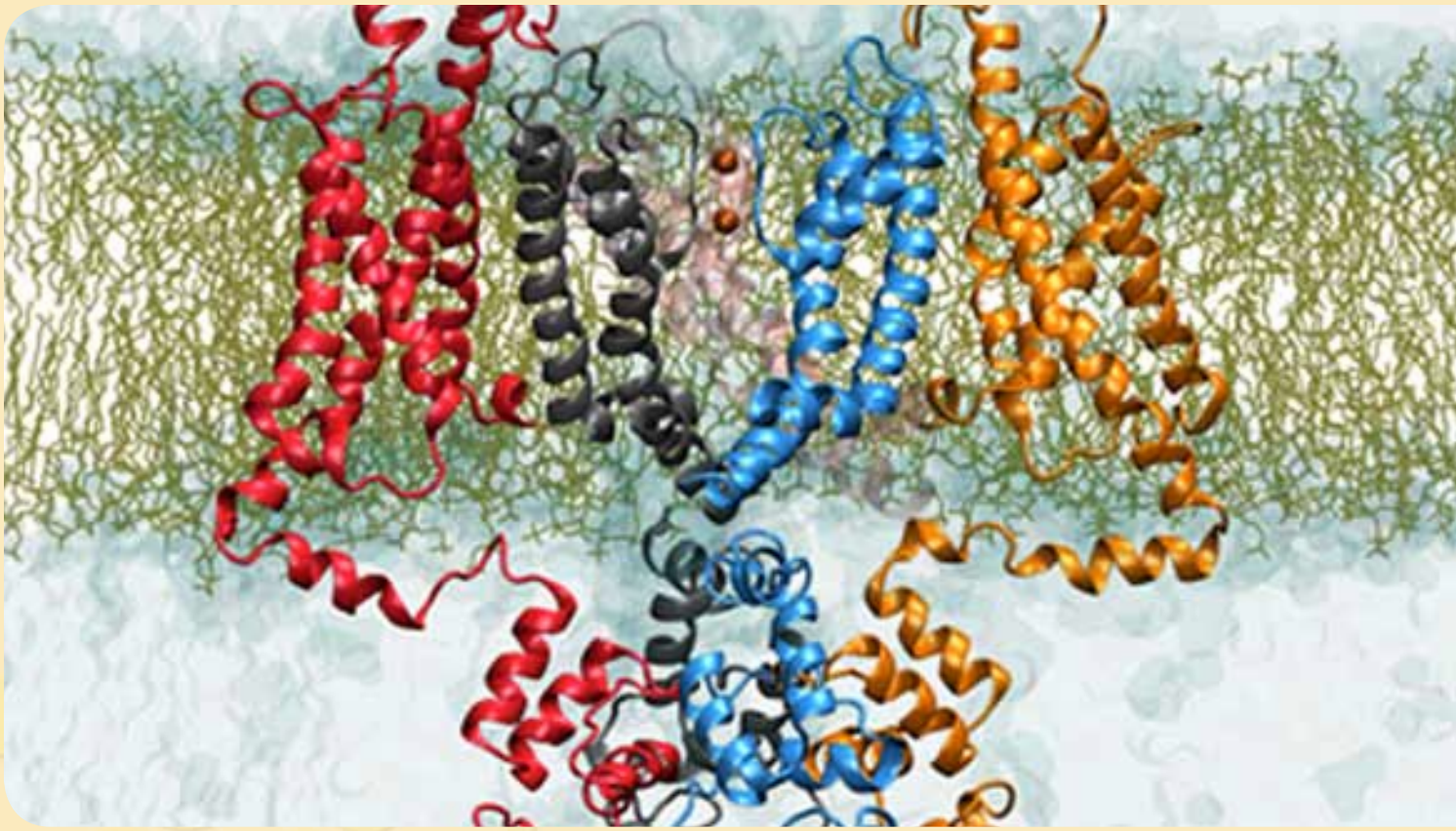
Paul Messina Appointed ALCF Director of Science

Dr. Paul Messina was appointed director of science at the ALCF. In this capacity, he guides the ALCF science teams using the IBM Blue Gene/P system and helps them achieve the best science output obtainable. Prior to this appointment, Messina acted as distinguished senior computer scientist at Argonne National Laboratory and adviser to the director general at CERN (European Organization for Nuclear Research).

ALCF Honored with Awards at SC08

The ALCF was recognized with several awards at SC08: The ALCF provided resources for Linear Scaling Divide-and-Conquer Electronic Structure Calculations for Thousand Atom Nanostructures, a collaborative effort between Lawrence Berkeley National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory that received the ACM Gordon Bell Prize Special Award (Algorithmic Innovation). ALCF staff members Paul Messina, Katherine Riley, and William Scullin addressed scaling and performance limitations and helped improve the performance of LS3DF on Intrepid.

The ALCF also was named a winner in two of the four categories in the HPC Challenge best performance benchmark competition, which were run using 32 racks of the Blue Gene/P. The ALCF's score of 103 GUPS (Giga Updates per Second) for Global RandomAccess was almost three times faster than last year's winner. The ALCF also won the Global FFT category, which measures the floating point rate of execution of double precision complex one-dimensional Discrete Fourier Transform, which is used to efficiently transform one function into another scoring 5,080 Gflops.



2008 RESEARCH DISCOVERIES

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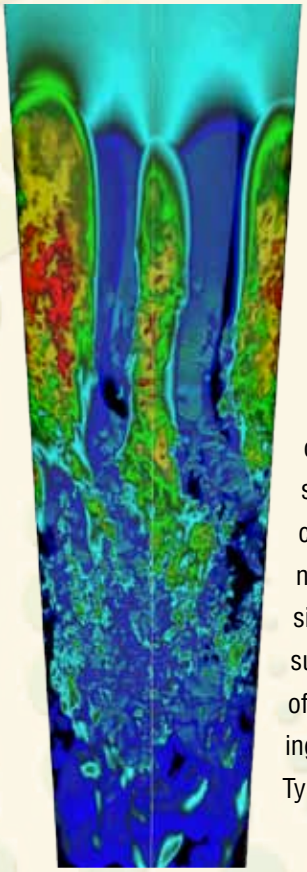
Applied Mathematics

Making Safe, Clean Nuclear Energy Available Globally

The United States is committed to new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global energy demand. Liquid-metal-cooled fast reactors are a key component of this strategy in that they permit recycling of nuclear fuel and are expected to be economical sources of power. A research team led by Paul Fischer of Argonne National Laboratory, comprised of researchers from Argonne and the University of Illinois, carried out large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores. The researchers simulated wire-wrapped fuel rods with 7-, 19-, and 37-pin bundles on the Blue Gene/P at the ALCF. The current computations are some of the largest to date with the spectral element code, Nek5000, and involve several hundred million gridpoints on unstructured meshes. Experiments indicated that low pin count results do not extrapolate to higher pin counts because of the edge channel effects. Succeeding simulations will involve more fuel pins, culminating in the design target of 217 pins. The simulations will enable researchers to gain an understanding of the fundamental thermal mixing phenomena within advanced recycling reactor cores, which can lead to improved safety and economy of these pivotal designs.

Astrophysics

Illuminating Scientists' Knowledge of the Universe



Led by Donald Lamb, NNSA ASC/Alliance Flash Center, The University of Chicago, researchers studied critical aspects of Type Ia supernovae, among the brightest and most powerful exploding stars in the universe. Type Ia create many of the elements from which we are made and are important for measuring distances in the universe. Two major challenges currently face Type Ia—1) buoyancy-driven turbulent nuclear burning, a key physical process in Type Ia, is not fully understood; and 2) few simulations of the four current models of Type Ia have been done. Working together, the researchers optimized the FLASH code to run efficiently on all 163,840 processors of the IBM Blue Gene/P supercomputer at the ALCF for buoyancy-driven turbulent nuclear burning simulations. They have run a grid of simulations for different physical conditions. The researchers also developed parallel processing tools needed to analyze the large amounts of data produced by the FLASH simulations. Preliminary analysis of these results showed that the flame surface is complex at large scales and smooth at small scales. The results of this work will be used to treat buoyancy-driven turbulent nuclear burning more accurately in the whole-star, three-dimensional simulations of Type Ia at the NNSA ASC/Alliance Flash Center.

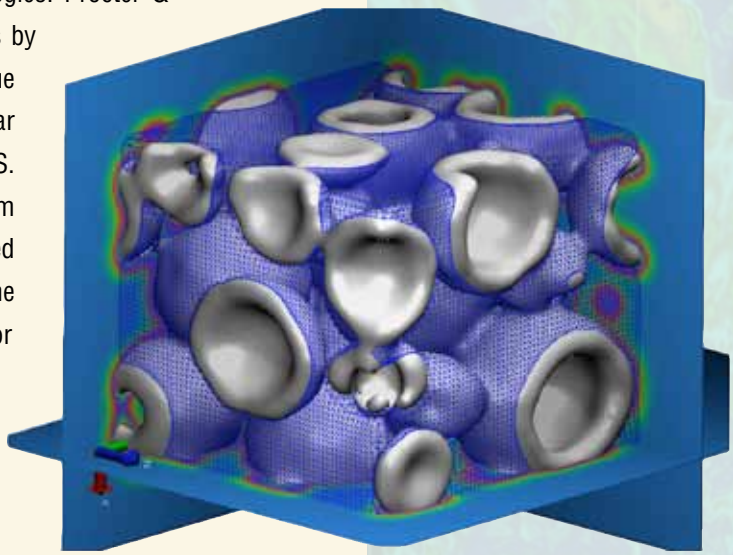
Chemical Sciences

Conducting Molecular Simulations of Complex Chemical Systems

Understanding reactions on a molecular scale is critical to solving many of the challenges facing the 21st century. Leadership class computing provides scientists with the computational molecular simulations of reactions that will lead to unprecedented discovery and will move the field of molecular simulation to a radically new simulation protocol. Led by Christopher Mundy, researchers at Pacific Northwest National Laboratory, in collaboration with IBM Research, applied statistical mechanical sampling methods in conjunction with density functional theory (DFT)-based interaction potentials to make detailed models of chemical processes at interfaces. The basic chemical physics of these leadership calculations will provide a detailed, molecular-scale picture of ions and reactions near interfaces. The researchers have obtained results on the free energies of transfer of OH^- and SO_2 from the bulk to interface. Through the direct simultaneous sampling of different reaction's coordinates, a picture is emerging where the structure and chemistry of species at interfaces differ dramatically from the bulk.

Enabling Breakthrough Innovation at P&G

Some of the world's most well-known and highly regarded industrial companies have sought out Argonne's computing capability and technical expertise to convert that knowledge into transformative products and technologies. Procter & Gamble (P&G), one of the 25 largest U.S. companies by revenue, is among them. P&G researchers used the Blue Gene/P system at the ALCF to investigate the molecular mechanisms of bubble formation in foams. Their U.S. Department of Energy INCITE allocation allowed them to perform computer simulations at an unprecedented scale on the dissolving of soap and foaming of suds. The researchers have developed coarse-grained models for two relevant surfactants. Ultimately, the work is expected to help P&G formulate products faster and more efficiently. That means the consumer wins by getting better products sooner, and at better value, than would have been possible using traditional methods.



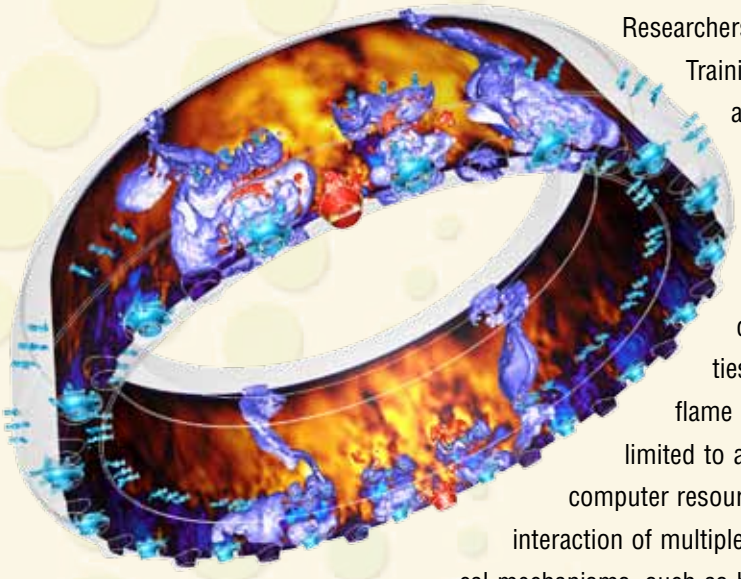
Climate Research

Developing Intricate Climate Models

Advanced computation, like that possible on the Blue Gene/P supercomputer at the-ALCF, allows researchers at the National Center for Atmospheric Research (NCAR) and U.S. Department of Energy (DOE) laboratories to develop more complex and intricate climate models. The vital information provided by these improved models will guide environmental policy. Using ALCF resources, the Climate Science Computational End Station advanced climate science through both an aggressive model development activity and an extensive suite of climate simulations, particularly the correct simulation of the global carbon cycle and its feedback to the climate system. The NCAR and DOE researchers tested a new, highly scalable method for solving the fluid dynamics of the atmosphere. This atmospheric Community Climate System Model component, called CAM/HOMME, has been shown to run with a resolution as high as 1/8 of a degree of latitude on over 80,000 cores. The research was led by Warren Washington, National Center for Atmospheric Research (NCAR), in collaboration with other researchers from NCAR, Argonne National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, NASA Headquarters, and Georgia Tech University.

Combustion

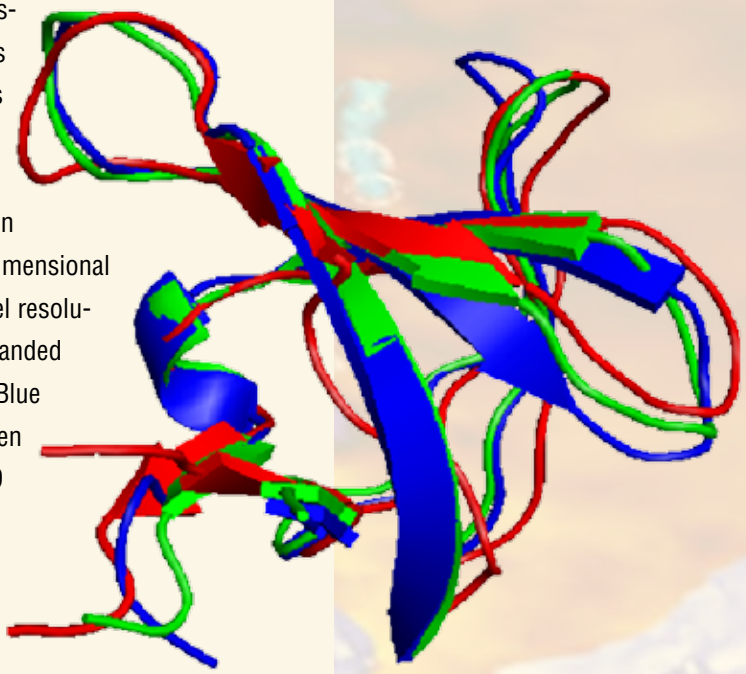
Focusing on Combustion in Gas Turbines



Researchers from the European Center for Research and Advanced Training in Scientific Computation (CERFACS) developed and applied the Large Eddy Simulation (LES) Computational Fluid Dynamics (CFD) approach for the simulation of unsteady reacting flows. Led by Thierry Poinsot, they focused on technically challenging issues in real gas turbines, thereby demonstrating the usefulness of LES in the design process. These issues, which are beyond the capacities of currently used CFD tools, include ignition, reignition, flame quenching, and instabilities. While CFD research is often limited to a single burner, combining LES and the massively parallel computer resources at the ALCF allowed the researchers to investigate the interaction of multiple burners in annular chambers and study important physical mechanisms, such as burner interactions, azimuthal acoustic modes generation, flame propagation from one burner to its neighbors, or how quenching occurs. Data gathered from this research will have real-world application in energy production (e.g., helicopter and aircraft engines).

Computational Proteomics

Predicting Structures of Biologically Important Proteins



Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires a detailed picture of their structure. To address this challenge, a research group led by David Baker at the University of Washington has developed and is using the ROSETTA method for computationally predicting protein structure. The group's goal was to create detailed, three-dimensional models of the structure of selected proteins at atomic-level resolution. Under the INCITE program, the team refined and expanded the capabilities of the ROSETTA method by using the Blue Gene/P at the ALCF. Over the past year, the method has been tested on several proteins of known structure up to 189 amino acids in length. In many cases, the accuracy of the prediction was within a remarkable one angstrom of the experimentally solved high-resolution crystal structure. The method was tested on proteins of known structure to determine the size range and fold classes for which accurate results can be predicted. Subsequent computations will focus on making predictions for proteins with unknown structures. Additional work will go into refining the method to expand the range of proteins to which it can be applied.

Computer Sciences

Developing a New Software Environment for Supercomputers

A team of researchers worked to provide a new software environment for supercomputers that makes the supercomputer appear to be part of the user's desktop system, instead of a remote and hard-to-access external computer. Initial work expanded the version of Plan 9 that was ported onto the BG/L system for the FASTOS program by Sandia National Laboratories, Bell Labs, IBM, and Vita Nuova. Led by Ronald Minnich, Sandia National Laboratories, the researchers tested all aspects of the Plan 9 environment and modified it as needed for large-scale machines.

Providing the Performance Community with Leadership Class Computing

The Performance Evaluation and Analysis Consortium (PEAC) End Station provides the performance community with access to the U.S. Department of Energy's leadership class computing facilities (LCF). The performance community, in turn, supports the centers and the computational scientists conducting research at these centers in many ways: developing performance tools and other performance-related infrastructure, characterizing performance and providing guidance on using the systems, and working directly with important simulation models. Recent results included the initial port of the Berkeley UPC compiler to the Blue Gene/P at the ALCF (available for download at http://upc.lbl.gov/download). The PEAC's INCITE allocation was also used in the performance analysis and optimization of a code that won a special ACM Gordon Bell Prize for algorithm innovation, presented at SC08, and in a SC08 paper on evaluating the promise of the BG/P architecture for computational science. Patrick Worley, Oak Ridge National Laboratory, led a team of researchers from Lawrence Berkeley National Laboratory, University of Tennessee, Argonne National Laboratory, University of Maryland, University of Oregon, Rice University, University of Wisconsin, University of North Carolina, University of California—San Diego, University of California—Berkeley, Oak Ridge National Laboratory, and Lawrence Livermore National Laboratory in the PEAC initiative.

Engineering Physics

Improving Aircraft Engine Combustor Simulations

A jet engine combustor combines air flowing faster than a hurricane with swirling fuel to generate the extraordinary release of heat that ultimately powers the aircraft. Understanding these complex physical and chemical interactions is critical to fuel efficiency and emissions performance, but physical testing can be difficult and time consuming. Pratt & Whitney (P&W) explored leading-edge combustor design methods using the Blue Gene/P supercomputer at the ALCF. This work studied the effect of different fidelities of analysis as well as computational methods to reduce turnaround time. The goal was to define a design process that made simulations that were traditionally challenging "one offs" usable in the production design cycle for next-generation commercial and military jet engines. The research has led to improved capabilities and reduced solution times for 3-D combustor simulations. It has been a key enabler for the depth of understanding needed to meet emissions goals. Capabilities improved through the INCITE allocations are now being applied to P&W's next-generation, low-emission PurePower™ engine.

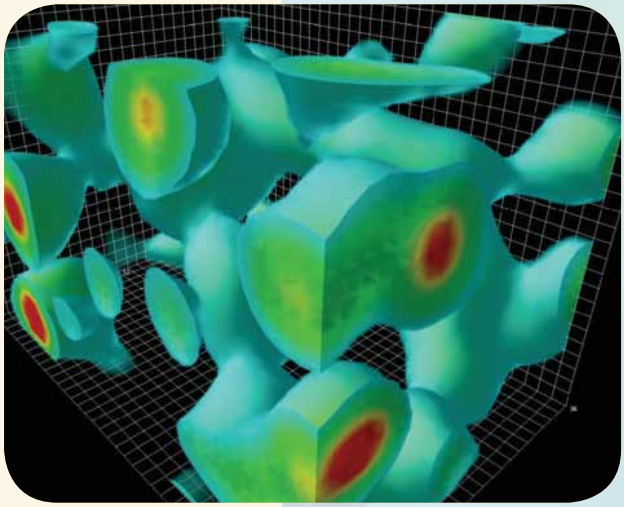
Fusion Energy

Simulating Plasma Microturbulence

Use of predictive computational models derived from first-principles physics equations has allowed for unparalleled gains in scientists' knowledge of microturbulence. Led by William Tang of the Princeton Plasma Physics Laboratory (PPPL), scientists from PPPL, Columbia University, and Oak Ridge National Laboratory have significantly enhanced the capabilities of a 3-D global particle-in-cell code (GTC) by employing a hybrid (Open MP/MPI) approach that has enabled more effective utilization of the ALCF's Blue Gene/P quad-core LCF. The BG/P's multi-core system now allows higher-resolution simulations in a multi-dimensional phase-space for conducting a realistic examination of the effect of collisions on plasma confinement properties. With this unprecedented capability, advanced kinetic simulations with higher physics fidelity can be directly applied for the systematic interpretation of experimental results in the near future. This, in turn, will help pave the way for scientific discoveries needed for accelerating progress towards the ultimate goal of attaining and harnessing essentially inexhaustible fusion power in the form of a secure and reliable energy system that is environmentally and economically sustainable.

Lattice Gauge Theory

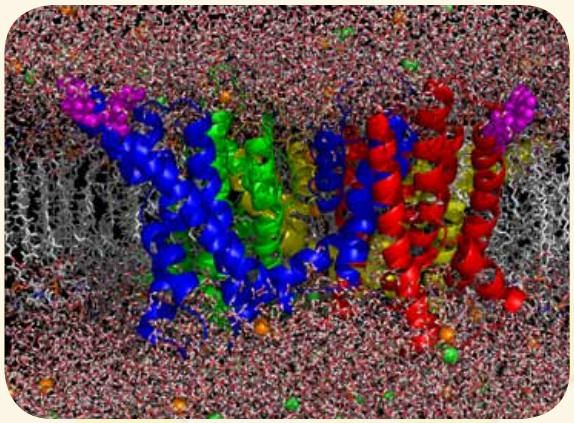
Understanding the Interactions between Quarks and Gluons



Scientists are seeking to increase their knowledge of the interactions between quarks and gluons, the basic constituents of 99% of the visible matter in the universe. Their research will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature. The scientists generated gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to their physical values found in nature. The Blue Gene/P at the ALCF has tremendously accelerated the generation of the gauge configurations—in many cases, by a factor of 5 to 10 over what has been possible with other machines. Significant progress has been made in simulations with two different implementations of the quarks—domain wall and staggered. The work will greatly improve the accuracy of the scientists' determination of a wide range of important quantities in high energy and nuclear physics. The project was led by Robert Sugar, University of California—Santa Barbara, in collaboration with researchers from Brookhaven National Laboratory, Massachusetts Institute of Technology, Thomas Jefferson National Accelerator Facility, University of Washington, Boston University, Fermi National Accelerator Laboratory, and Columbia University.

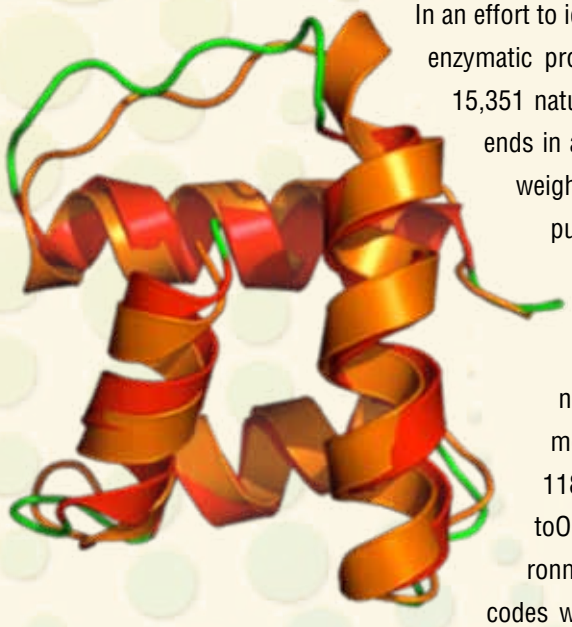
Life Sciences

Breaking New Ground in Membrane Protein Research



Numerous biological processes are controlled by proteins in the cell membrane, ranging from production of biofuels to cleaning up toxic organic waste. Large-scale gating motions, occurring on a relatively slow time scale, are essential for the function of many important membrane proteins such as transporters and channels. Voltage-activated ion channels are literally electric switches that are turned "on" by a change in the cellular potential. Malfunction of those channels can lead to cardiac arrhythmia and neurological pathologies. Led by Benoit Roux, Argonne National Laboratory and The University of Chicago, in collaboration with researchers from the University of Illinois, Urbana-Champaign, the research team used high-performance computing to break new ground in understanding how these membrane proteins work. Exploiting state-of-the-art developments in molecular dynamics and protein modeling, the team constructed models of voltage-gated potassium channels and ran them on the ALCF's Blue Gene/P and Oak Ridge National Laboratory's CRAY XT leadership-class computers, using INCITE resources. An important result of these simulations concerned the properties of the electric field responsible for the voltage activation. The calculations showed that this electric field was indeed more intense than at other equivalent positions across the membrane far away from the protein. These results opened up the possibility of better-designed therapeutic drugs, as well as the construction of artificial biomemetic nano-switches.

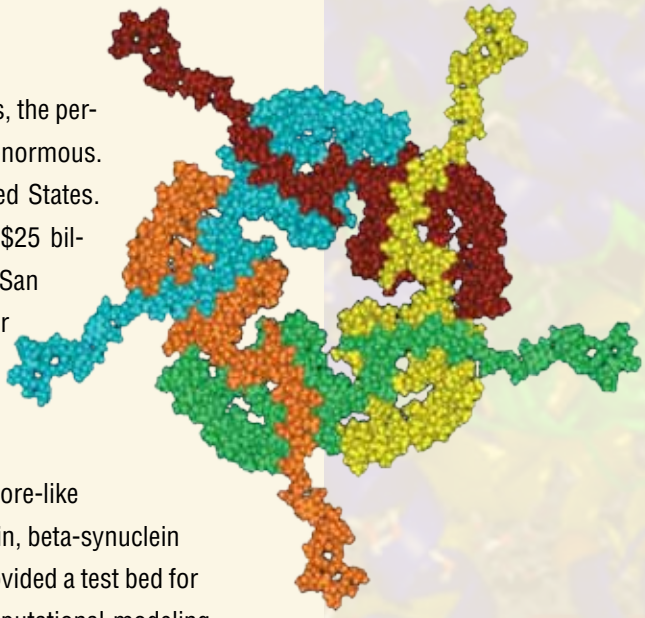
Identifying Potential Drug Targets



In an effort to identify potential drug targets, Argonne researchers screened nine enzymatic proteins in the core metabolism of bacteria and humans against 15,351 natural compounds and existing drugs. They aimed to reduce dead ends in antibiotics and anticancer drugs. The researchers used the lightweight, multilevel task scheduler, Falkon, running on the ZeptoOS compute node kernel, to manage the run on the IBM Blue Gene/P at the ALCF. Falkon enables the rapid dispatch of independent tasks to any BG/P compute node core in milliseconds. It can dispatch over a thousand tasks per second, keeping all BG/P compute nodes fully utilized, even when running a workload of a million or more relatively short, or varying length tasks. In one such example, 118,000 cores were used running nearly one million tasks. The ZeptoOS operating system provides Falkon with a complete Linux environment in which to transparently execute most scientific applications codes with little or no change. The potentially huge demand that such

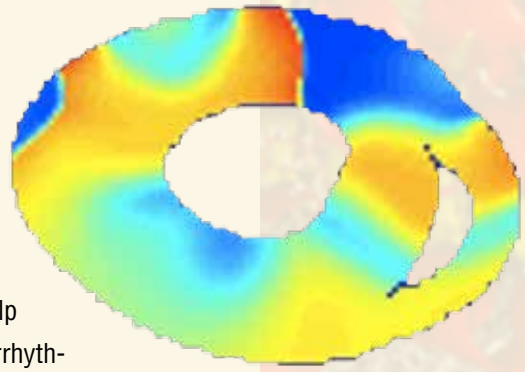
a computing approach—called "many-task computing"—could place on the BG/P I/O system was reduced by careful caching and batching of file operations. Recent research has aimed at automating this manual I/O tuning through a general-purpose parallel scripting language called Swift. Despite the challenges of taking many-task computing to petascale performance levels, researchers completed 21.43 CPU-years of analysis in 2.01 wall-hours.

Modeling the Molecular Basis of Parkinson's Disease



As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Currently, there are more than 2 million cases in the United States. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone. University of California—San Diego scientists leveraged the high-end computation power of the Blue Gene/P at the ALCF to learn more about the molecular basis of the disease and explore ways to treat it. They have found that the clumping of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes. In contrast, another protein, beta-synuclein (bS), appears to block the clumping action. The findings provided a test bed for identifying possible therapeutic interventions through computational modeling. Given the encouraging correlation between their molecular dynamics modeling predictions and laboratory experimental results, the team expected to make steady progress both with the computational model itself, as well as with the design of effective drugs based on the computational modeling and simulations.

Preventing Cardiac Rhythm Disorders

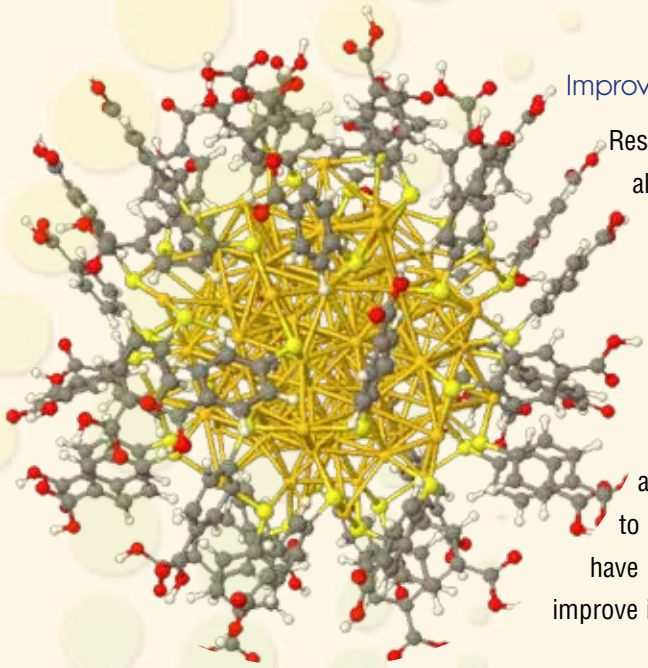


In work funded by the National Institutes of Health, a research team led by Jeffrey Fox, Cornell University, used the Blue Gene/P at the ALCF to rapidly test hypotheses for the initiation and maintenance of cardiac rhythm disorders. The team's large-scale computer simulations represented a promising tool to help identify the underlying electrical mechanisms for dangerous arrhythmias and determine the effects of interventions, such as drugs, that may prevent or exacerbate these arrhythmias. Certain activation sequences have been shown to be particularly effective at inducing arrhythmias in canine experimental models. The research team showed that similar sequences induce wave break, reentry, and sustained fibrillatory activity in a 3-D model of electrical wave propagation in the canine heart.

MATERIALS SCIENCE

Accelerating the Pace of Discovery in Alternative Fuels Research

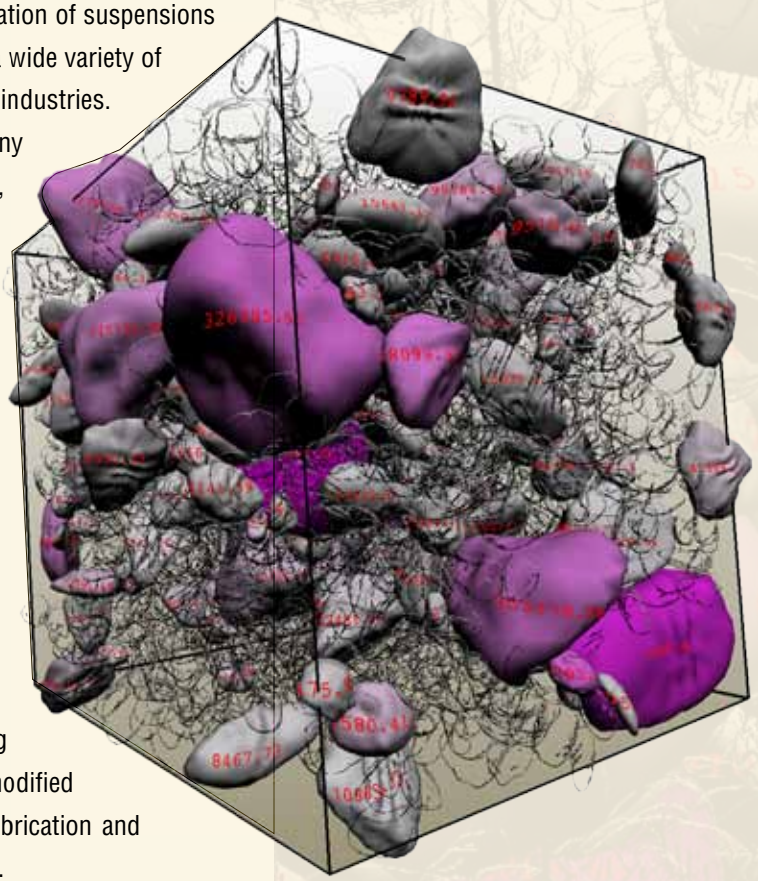
Scientists continue to seek clean, renewable energy sources that will reduce our dependence on foreign oil. One promising possible energy source for cars is hydrogen. However, currently available methods of storing hydrogen in materials are typically either much too heavy or else bind the hydrogen within the material much too strongly. Quickly extracting hydrogen out of those materials requires extremely high levels of heat—impractical for actual use in vehicles on the open road. In research led by Christopher Wolverton at Northwestern University, in collaboration with the University of California—Los Angeles, researchers have recently developed a suite of computational materials science tools aimed at the discovery of novel hydrogen storage materials. The suite is based on first-principles methods that start with a quantum-mechanical description of the interaction of electrons in a solid. Using the Blue Gene/P at the ALCF, the novel tools allow the prediction of the thermodynamic conditions under which hydrogen can be inserted and removed from a given material, while also predicting the new atomic-scale crystal structure of the predicted material. These capabilities have led to the prediction of several novel, high-density hydrogen storage materials and reactions.



Improving Software Performance on the Blue Gene/P

Researchers from the ALCF, Argonne's Center for Nanoscale Materials (CNM), the Technical University of Denmark, and University of Copenhagen collaborated to work on GPAW, a software package for performing density functional calculations, a quantum mechanical method for computing the properties of matter. The collaboration's primary goal was to improve the performance of GPAW on the IBM Blue Gene/P at the ALCF, and to this end, enable the CNM to characterize next-generation catalytic materials. An additional layer of parallelization is needed to scale GPAW to a larger number of nodes on the Blue Gene/P. The researchers have implemented an initial version of this algorithm and continue to improve it. Progress also was made on related performance improvements.

Modeling the Rheological Properties of Concrete



Understanding the mechanisms for the dispersion or agglomeration of suspensions remains a great challenge and has technological application in a wide variety of areas, including the pharmaceutical, food, coatings, and building industries. Yield stress is a well-known but not understood property of many fluids, including cement-based materials (cement paste, mortars, and concrete). It is often thought of as the maximum force needed to break bonds in colloidal materials. However, analysis of the simulation data of dense suspension has shown that an important cause of yield stress is a supplementary stress that develops at the onset of flow. This supplementary stress is due to the organization of the contacts of aggregates in the compression quadrant, as stress is distributed throughout the suspension when it is sheared, and it is not accounted for by the simple breaking of bonds assumed in most theories of yield stress. This important discovery should affect how admixture companies design their products to mitigate this effect and reduce energy costs. William George led a group of researchers from the National Institute of Standards and Technology in using a computational approach for this research that is based on a modified Dissipative Particle Dynamics (DPD) model, which includes lubrication and Van der Waals forces for different-shaped particles near contact.

Nuclear Energy

Predicting Thermal Striping in Sodium-Cooled Reactors

Computer simulation is aiding the design optimization of a new generation of Advanced Recycling Reactors (ARR). These reactors will be used to greatly reduce the amount of spent fuel storage required by light water reactors. A critical issue in the design of sodium-cooled fast reactors is predicting the phenomenon of "thermal striping"—when partially mixed streams of sodium coolant expose structural materials to cyclic thermal stresses that cause fatigue and limit their lifetime. Traditionally, designers have relied on data from instrumented experiments, but this data is expensive and difficult to collect and greatly limited in its spatial fidelity and adaptability to scope design space. Led by Andrew Siegel, Argonne National Laboratory researchers used INCITE resources to carry out the first detailed numerical experiments of thermal striping on realistic reactor geometries.

Nuclear Physics

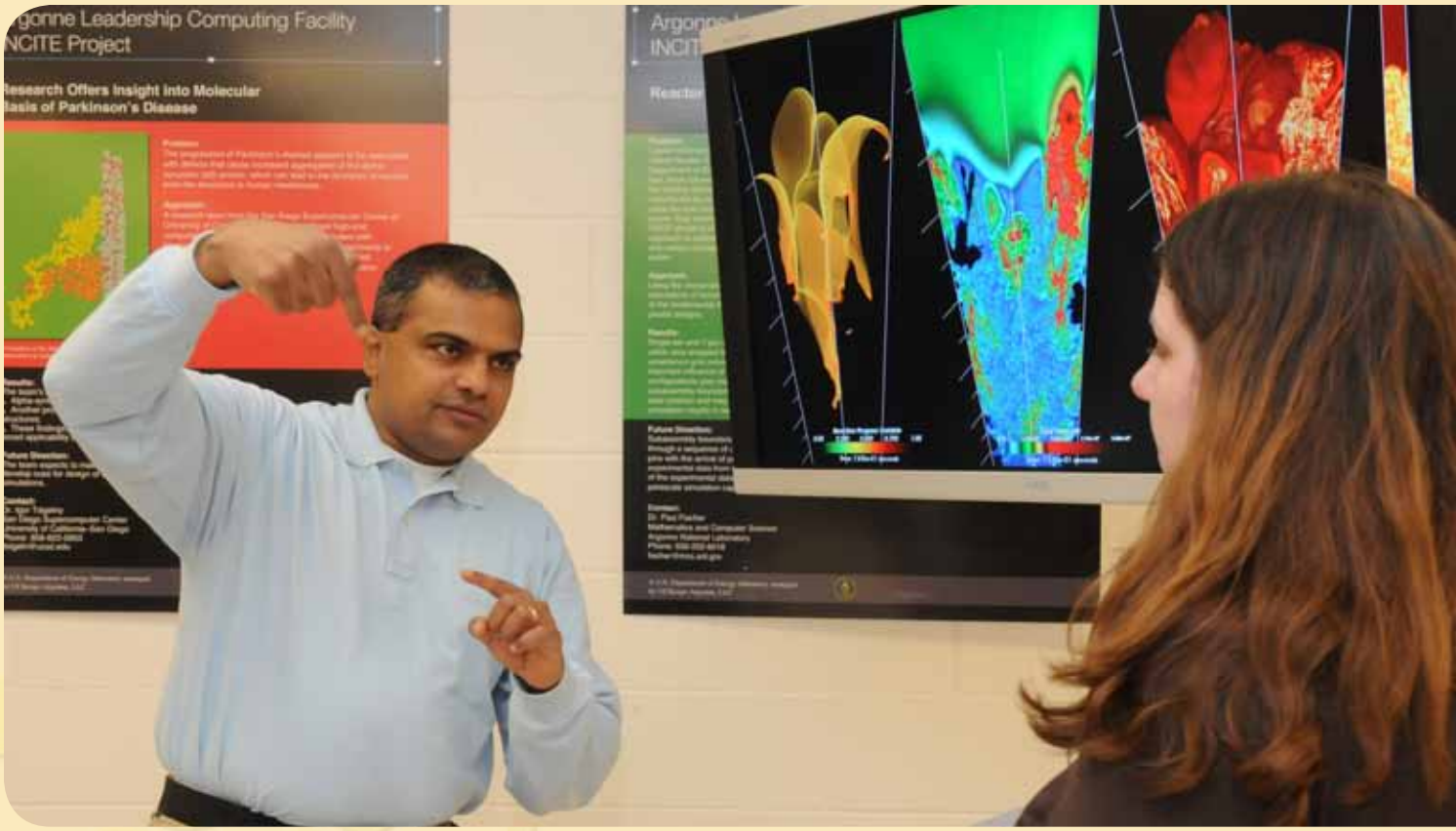
Exploring Nuclear Structure

Researchers used complementary techniques, including Green's Function Monte Carlo, Hamiltonian Diagonalization (the No Core Shell Model), and Coupled-Cluster methods to perform *ab initio* calculations of both structural and reaction properties of light and medium mass nuclei and the three-nucleon force. They conducted the calculations on the Cray XT4 at Oak Ridge National Laboratory and the IBM Blue Gene/P at the ALCF. Their work could provide an *ab initio* understanding of triple-alpha burning that is essential to life on earth. The project explored, for the first time, the role of the three-nucleon force in substantially heavier nuclei such as 160, 40Ca, and 56Ni. The research team was led by David Dean, Oak Ridge National Laboratory, in collaboration with researchers from Iowa State University, University of Tennessee, and Argonne National Laboratory.

Physical Chemistry

Probing the Properties of Water

Unraveling the properties of water at organic and inorganic interfaces is a key step towards understanding the function of biological systems and the behavior of soft and hard materials in many natural environments. Probing such properties is a very challenging task, both from an experimental and theoretical standpoint. The challenge is even greater if water is confined in very small spaces—within a few nanometers. Exploiting the power of IBM Blue Gene supercomputers at the ALCF and IBM Blue Gene Watson Research Laboratory, a team of researchers used first-principles simulations to investigate what happens at the microscopic level when water meets hydrophilic and hydrophobic surfaces and how the properties of this ubiquitous liquid are modified at the nanoscale. The first-principles theory used—density functional theory—yielded results that compare well with experiments for all the major structural properties of water, some of its electronic spectroscopic signatures, and several dynamical properties. In addition, the team identified the key role played by electrons in determining the arrangements of water molecules at the surface. They also computed vibrational spectra and provided predictions and interpretations of what should be seen experimentally when measuring how water molecules vibrate in contact with surfaces. The findings can be applied to solve complex problems in both biology and materials science.



ALCF OUTREACH

ALCF Workshops Provided Hands-on Help to Users

The Argonne Leadership Computing Facility (ALCF) held the following series of INCITE and Blue Gene/P (BG/P) workshops in 2008, starting with an Introduction to BG/P Workshop on February 20.

The March 4-5 INCITE Getting Started Workshop was attended by team members from 14 of the 20 INCITE projects at the ALCF. By the workshop's conclusion, all teams present had made meaningful forward strides. With few exceptions, nearly all the teams had code running on the Blue Gene/P and left the workshop ready to move into the next phase of scaling and performance tuning. Additionally, the INCITE project teams made preparations to begin their science runs on the 100-teraflops Blue Gene/P at the ALCF by the end of March.

The March 6 Introduction to the Blue Gene/P Workshop for Blue Gene Consortium members introduced researchers to the architecture and capabilities of the BG/P, as well as provided hands-on assistance for coding, porting, and tuning. It was jointly hosted by the ALCF and the Blue Gene Consortium. One attendee remarked about his scaling results for 32-molecule and 256-molecule water benchmarks running on the ALCF BG/P Surveyor system: "Notably, the 256 results are about twice as fast as on the Blue Gene/L. Blue Gene/P's superior network really shines in this benchmark. We feel this promises excellent scaling." Several researchers in attendance at the workshop successfully ported and tuned their applications with the help of both ALCF and IBM staff.

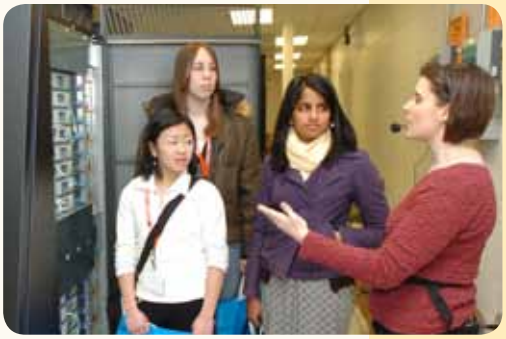
The ALCF offered an advanced INCITE Performance Workshop for DOE INCITE users on May 7-8 at Argonne. Thirty people attended the workshop. Advanced users received hands-on training on performance and debugging tools to enhance application performance and scalability on the Blue Gene/P. Feedback from the attendees indicated they found information and presentations about the profiling tools and parallel I/O to be especially useful.

In summer, 26 attendees learned about the petascale resources available to them at the Leap to Petascale Workshop on July 29-31. During the workshop, IBM and ALCF performance engineers helped workshop participants scale and tune their applications on the Blue Gene/P computer. Noted one participant, "Being able to interact and work on our problems with the technical staff was the best and most unique opportunity

of this workshop." Sponsors included the ALCF, Blue Gene Consortium, and Argonne National Laboratory.

The Blue Gene Consortium Open Source Workshop held August 12-13 at Argonne gave consortium members an understanding of the BG/P open source community organization and business model. It covered ongoing and potential research activities, described IBM's involvement, and allowed participants to brainstorm on future activities. Sponsors included the BG Consortium, Argonne Mathematics and Computer Science Division, ALCF, and IBM.

Students Toured ISSF at Science Careers in Search of Women Conference



The annual Science Careers in Search of Women conference on April 3 brought high school women from 60 Chicago-area schools to Argonne to experience science careers firsthand through interactions with female scientists. Approximately 20 students toured the ALCF's Interim Supercomputing Support Facility (ISSF) and got a close-up look at the Blue Gene/P supercomputer, accompanied by tour leader Sandra Bittner, Senior UNIX Security Engineer, and Chel Lancaster, Marketing and Outreach Coordinator at the ALCF.

Supercomputing Careers Highlighted at Collegiate Scholars Career Roundtable

At the annual career roundtable hosted by The University of Chicago Collegiate Scholars Program (CSP) and Goldman Sachs on April 5, the ALCF's Ira Goldberg met with Chicago Public High School students to discuss careers in supercomputing. The event was part of an array of enriching college-preparatory opportunities CSP offers students (http://collegiatescholars.uchicago.edu). CSP's goal is to prepare talented students for academic success at the best colleges and universities.

ALCF Held Open House for Argonne, DOE, The University of Chicago Employees

Approximately 350 Argonne, U.S. Department of Energy, and The University of Chicago employees attended an open house hosted by the ALCF on August 14. The ALCF is home to Intrepid, IBM's next-generation Blue Gene/P system, with a peak speed of 557 teraflops. The open house provided employees with an overview of the ALCF and a tour of the supercomputing support facility.

Argonne's Computational Research Highlighted at Grace Hopper Celebration

Argonne staff discussed computational research in progress at the ALCF and Mathematics and Computer Science Division with attendees at the Grace Hopper Celebration of Women in Computing on October 1-4 at the Keystone Resort, Colorado. Argonne representatives also provided information on the latest job opportunities. The Grace Hopper Celebration offered a series of conferences designed to bring the research and career interests of women in computing to the forefront. Leading researchers presented their current work, while special sessions focused on the role of women in today's technology fields, including computer science, information technology, research and engineering. Past Grace Hopper Celebrations have resulted in collaborative proposals, networking, mentoring, and increased visibility for the contributions of women in computing.

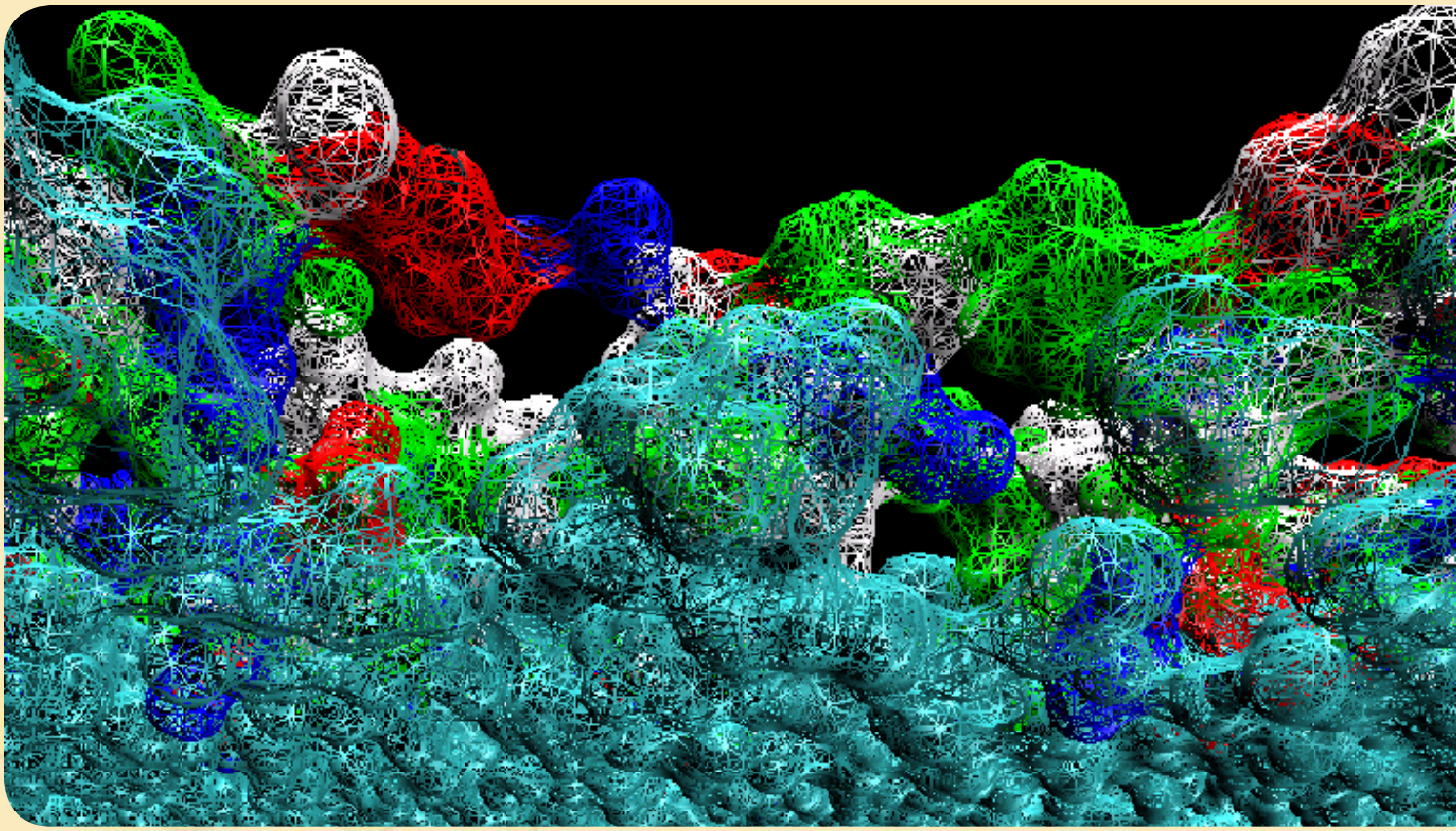
Why Choose a Career in Scientific Computing?

William Scullin, Senior HPC Systems Administrator at the ALCF, explained to students why they should consider a career in scientific computing at the 2008 ACM South Central Programming Contest (http://acm2008.cct.lsu.edu/sites/lsu/) on October 17. He gave an invited presentation to undergraduate students and coaches about scientific computing research under way and opportunities that are available to students at the ALCF.

Staff Highlighted ALCF's Breakthrough Science at SC08

At SC08, Argonne staff participated in a whole host of activities that highlighted the breakthrough science being conducted at the ALCF. Staff members were involved in tutorials, papers, panels, posters, workshops, demos and presentations, as well as SC committees at the conference, held November 15-21 in Austin, Texas. The Argonne booth showcased a diverse range of breakthrough science and engineering endeavors enabled by the ALCF's world-leading computing capability. The full list of activities can be found on the web (http://www.cels.anl.gov/events/conferences/SC08/).

In addition, staff members hosted four Birds-of-a-Feather (BOF) sessions at the SC08 conference. On November 18, Pete Beckman, ALCF Director, led a session on "Coordinated Fault Tolerance in High-End Computing Environments." Susan Coghlan, ALCF Associate Division Director, facilitated another BOF on the "Blue Gene System Management Community." This session provided an opportunity for Blue Gene system administrators to share information and discuss problems. On the same day, Kalyan Kumaran, ALCF Manager, Application Performance Engineering and Data Analytics, presented a BOF on "SPEC MPI2007: A Benchmark to Measure MPI Application Performance." His talk described the benchmark creation process and a roadmap of future additions to the suite. On November 19, Katherine Riley, ALCF Team Lead, Catalyst, facilitated a fourth session on "Petascale Computing Experiences on Blue Gene/P." Kalyan Kumaran and Paul Messina, ALCF Director of Science, also spoke at this session. With well over 100 applications ported to the Blue Gene/P at the ALCF, many lessons were shared.



2009 INCITE RESEARCH PROJECTS

Applied Mathematics
Reactor Core Hydrodynamics
Paul Fischer, Argonne National Laboratory
INCITE Hours Allocation: 30,000,000

Astrophysics
Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernovae Models
Don Lamb, NNSA ASC/Alliance Flash Center The University of Chicago
INCITE Hours Allocation: 70,000,000

Biological Sciences
Sculpting Biological Membranes by Proteins
Klaus Schulten, University of Illinois
INCITE Hours Allocation: 9,240,000

Biological Sciences
Simulation and Modeling of Membrane Interactions with Unstructured Proteins and Computational Designs of Membrane Channels for Absorption of Specified Ions
Igor Tsigelny, University of California–San Diego
INCITE Hours Allocation: 3,000,000

Chemical Sciences
Molecular Simulation of Complex Chemical Systems
Christopher Mundy, Pacific Northwest National Laboratory
INCITE Hours Allocation: 2,000,000

Chemical Sciences
Molecular Simulations of Surfactant-Assisted Aqueous Foam Formations
Kelly Anderson, Procter and Gamble
INCITE Hours Allocation: 6,000,000

Chemical Sciences
Water in Confined States
Giulia Galli, University of California–Davis
INCITE Hours Allocation: 2,000,000

Climate Research
Climate-Science Computational End Station Development and Grand Challenge Team
Warren Washington, National Center for Atmospheric Research
INCITE Hours Allocation: 7,500,000

Climate Research
Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence
Susan Kurien, Los Alamos National Laboratory
INCITE Hours Allocation: 25,000,000

Climate Research
The Role of Eddies in the Meridional Overturning Circulation
Paola Cessi, Scripps Institution of Oceanography/University of California–San Diego
INCITE Hours Allocation: 5,000,000

Combustion
Massively Parallel Simulation of Combustion in Gas Turbines
Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
INCITE Hours Allocation: 8,000,000

Computational Proteomics
Computational Protein Structure Prediction and Protein Design
David Baker, University of Washington
INCITE Hours Allocation: 12,000,000

Computer Sciences
Blue Gene/P Plan 9 Measurements on Large-Scale Systems
Ronald Minnich, Sandia National Laboratories
INCITE Hours Allocation: 8,000,000

Computer Sciences
Performance Evaluation and Analysis Consortium End Station
Patrick Worley, Oak Ridge National Laboratory
INCITE Hours Allocation: 8,000,000

Engineering
Fundamental Study of Shock/Turbulence Interaction
Sanjiva Lele, Stanford University
INCITE Hours Allocation: 8,000,000

Engineering
Petascale Adaptive CFD for Anisotropic Flows
Kenneth Jansen, Rensselaer Polytechnic Institute
INCITE Hours Allocation: 5,000,000

Environmental Sciences

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz

Thomas Jordan, Southern California Earthquake Center
INCITE Hours Allocation: 5,000,000

Fusion Energy

High-Resolution Global Simulation of Plasma Microturbulence

William Tang, Princeton Plasma Physics Laboratory
INCITE Hours Allocation: 6,000,000

Lattice Gauge Theory

Lattice QCD

Paul Mackenzie, Fermi National Accelerator Laboratory
INCITE Hours Allocation: 67,000,000

Life Sciences

Gating Mechanism of Membrane Proteins

Benoit Roux, Argonne National Laboratory and The University of Chicago
INCITE Hours Allocation: 30,000,000

Life Sciences

Large-Scale Simulations of Cardiac Electrical Activity

Jeffrey Fox, Cornell University
INCITE Hours Allocation: 21,405,500

Materials Science

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles

Christopher Wolverton, Northwestern University
INCITE Hours Allocation: 1,000,000

Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations

Peter Coveney, University College London
INCITE Hours Allocation: 40,000,000

Materials Science

Linear Scale Electronic Structure Calculations for Nanostructures

Lin-Wang Wang, Lawrence Berkeley National Laboratory
INCITE Hours Allocation: 1,000,000

Materials Science

Modeling the Rheological Properties of Concrete

William George, National Institute of Standards and Technology
INCITE Hours Allocation: 750,000

Nuclear Energy

Predictions of Thermal Striping in Sodium–Cooled Reactors

Andrew Siegel, Argonne National Laboratory
INCITE Hours Allocation: 7,500,000

Nuclear Physics

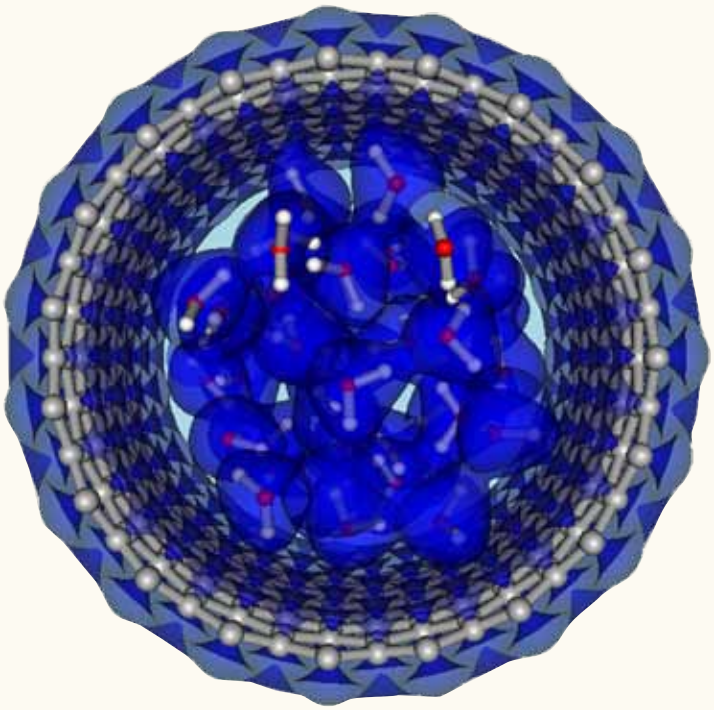
Computational Nuclear Structure

David Dean, Oak Ridge National Laboratory
INCITE Hours Allocation: 10,000,000

Plasma Physics

Three-Dimensional Particle-in-Cell Simulations of Fast Ignition

Chuang Ren, University of Rochester
INCITE Hours Allocation: 1,500,000



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