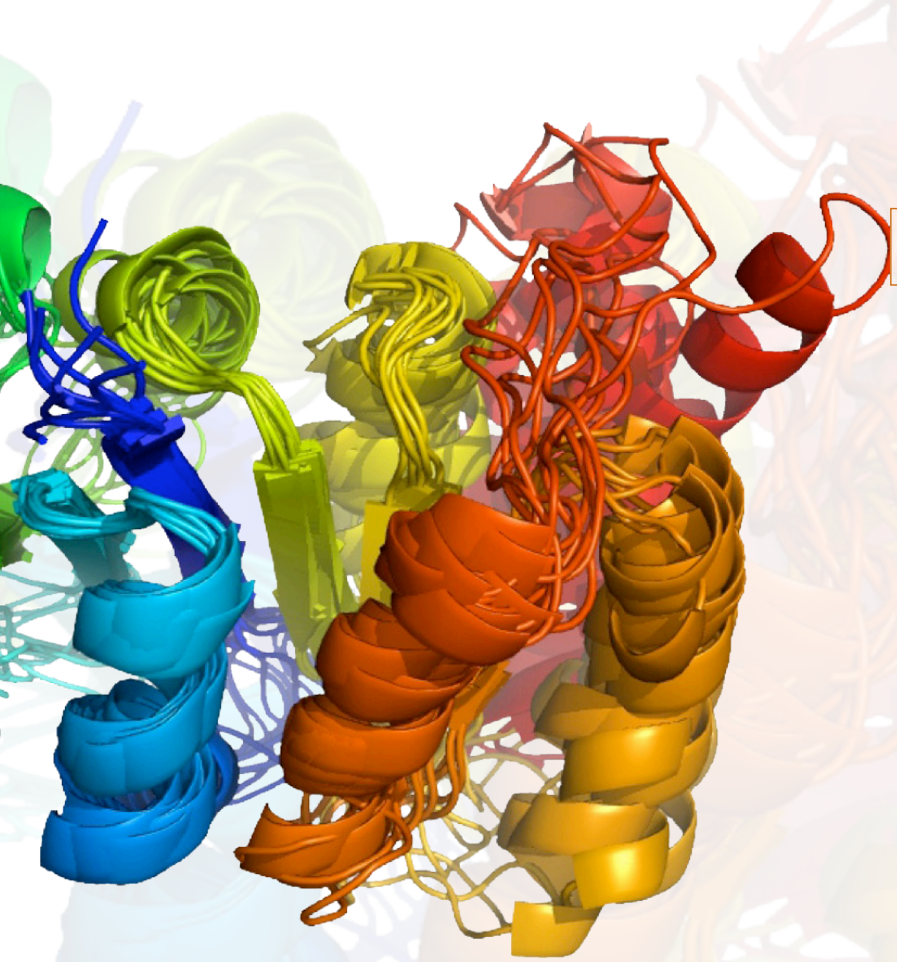

Argonne NATIONAL LABORATORY | Argonne Leadership Computing Facility

Argonne Leadership Computing Facility

ANNUAL REPORT 2009

SOLVING SCIENTIFIC CHALLENGES THROUGH SUPERCOMPUTING

On the cover
Researchers determined this large protein, ALG13, which is 200 amino acids in length, with a new methodology called "NMR structure determination without side-chain assignments." (David Baker, University of Washington)

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Director's Message

Solving Scientific Challenges through Supercomputing

This year the Argonne Leadership Computing Facility (ALCF) delivered nearly 900 million core hours of science. The research conducted at our leadership class facility touched our lives in both minute and massive ways—whether it was studying the catalytic properties of gold nanoparticles, predicting protein structures, or unearthing the secrets of exploding stars.

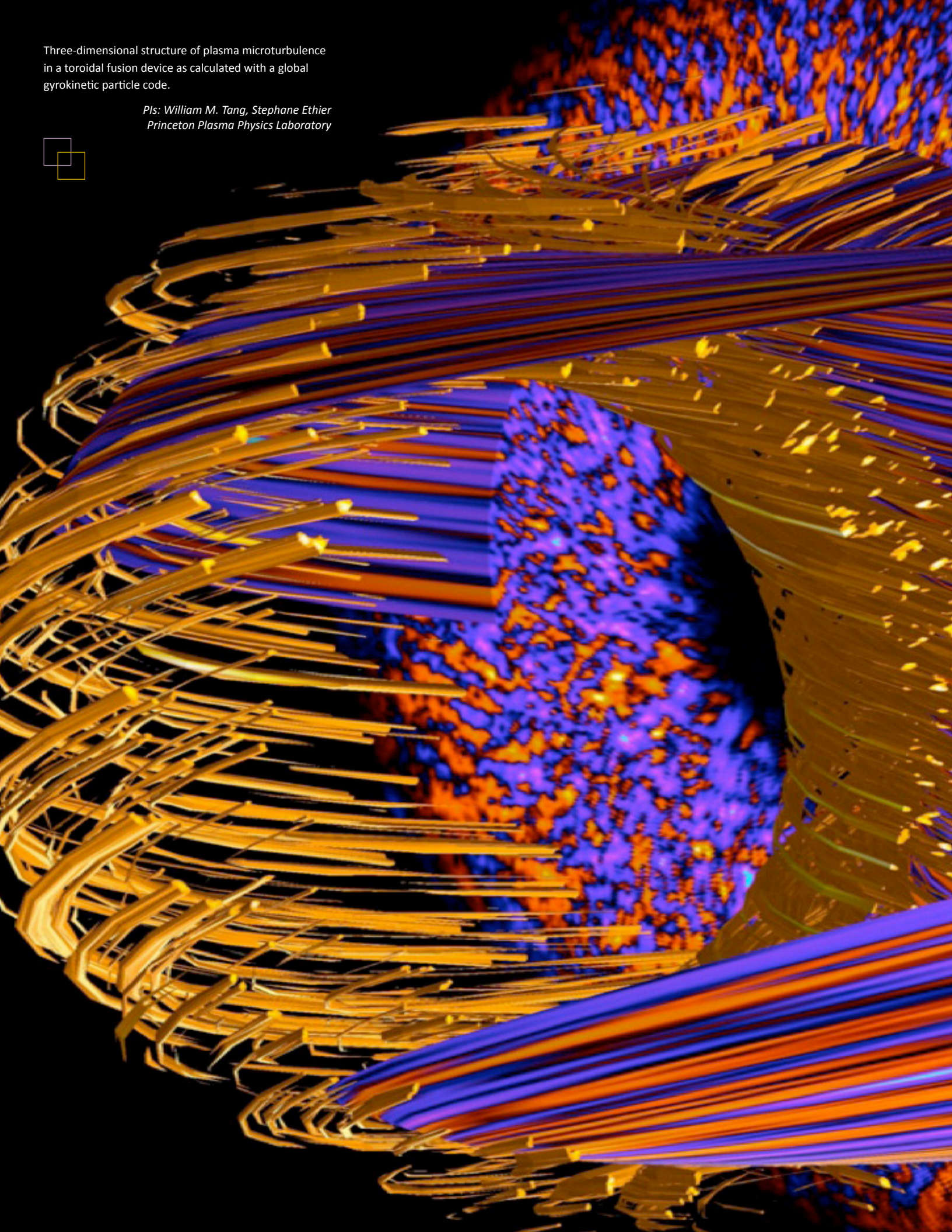
We remained true to our vision to act as the forefront computational center in extending science frontiers by solving pressing problems for our nation. Our success in this endeavor was due mainly to the Department of Energy's (DOE) INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. The program awards significant amounts of computing time to computationally intensive, unclassified research projects that can make high-impact scientific advances. This year, DOE allocated 400 million hours of time to 28 research projects at the ALCF. Scientists from around the world conducted the research, representing such esteemed institutions as the Princeton Plasma Physics Laboratory, National Institute of Standards and Technology, and European Center for Research and Advanced Training in Scientific Computation. Argonne also provided Director's Discretionary allocations for research challenges, addressing such issues as reducing aerodynamic noise, critical for next-generation "green" energy systems.

Intrepid—the ALCF 's 557-teraflops IBM Blue/Gene P supercomputer—enabled astounding scientific solutions and discoveries. Intrepid went into full production five months ahead of schedule. As a result, the ALCF nearly doubled the days of production computing available to the DOE Office of Science, INCITE awardees, and Argonne projects. One of the fastest supercomputers in the world for open science, the energy-efficient system uses about one-third as much electricity as a machine of comparable size built with more conventional parts. In October 2009, President Barack Obama recognized the excellence of the entire Blue Gene series by awarding it the National Medal of Technology and Innovation.

Other noteworthy achievements included the ALCF's collaboration with the National Energy Research Scientific Computing Center (NERSC) to examine cloud computing as a potential new computing paradigm for scientists. Named Magellan, the DOE-funded initiative will explore which science application programming models work well within the cloud, as well as evaluate the challenges that come with this new paradigm.

And the ALCF obtained approval for its next-generation machine, a 10-petaflops system to be delivered in 2012. This system will allow us to resolve ever more pressing problems, even more expeditiously through breakthrough science in the years to come.

Pete Beckman
Director
Argonne Leadership Computing Facility



Three-dimensional structure of plasma microturbulence in a toroidal fusion device as calculated with a global gyrokinetic particle code.

PIs: William M. Tang, Stephane Ethier
Princeton Plasma Physics Laboratory

OVERVIEW

ALCF Provides the Science Community with Leadership-Class Computing

Argonne operates the Argonne Leadership Computing Facility (ALCF) for the U.S. Department of Energy's (DOE) Office of Science as part of the larger DOE Leadership Computing Facility strategy. DOE leads the world in providing the most capable civilian supercomputers for science. Argonne researchers work closely with researchers from companies and universities, as well as federal, state, and municipal agencies to help them solve their specific problems, advance America's scientific leadership, and prepare the nation for a better future.

Mission

The Argonne Leadership Computing Facility's (ALCF) mission 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.

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.

ALCF Timeline

2004
- Formed the Blue Gene Consortium with IBM

2005
- Installed 5-teraflops Blue Gene/L for evaluation

2006
- Began production support of 6 INCITE projects
- Continued code development and evaluation

2007
- Increased to 9 INCITE projects
- Continued development projects
- Held Next Generation Blue Gene workshop (June)
- Installed 100-teraflops Blue Gene/P (Oct.-Nov.)
- Accepted 100-teraflops Blue Gene/P (Dec.)

2008
- Increased to 20 INCITE projects
- Began support of Early Science and INCITE projects on Blue Gene/P

2009
- Brought the 557-teraflops Blue Gene/P system into full production
- Began support of 28 INCITE projects
- Received approval for 10-petaflops system to be delivered in 2012 timeframe
- Began joint Argonne/NERSC Magellan cloud project
- Delivered 897M core hours of science

ALCF Leadership

Pete Beckman

Laural Briggs

Paul Messina

Susan Coghlan

Darin Wills

Ira Goldberg

David Martin

Kalyan Kumaran

Bill Allcock

Katherine Riley

Mark Hereld

Research and Resources

Major research endeavors are 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. 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

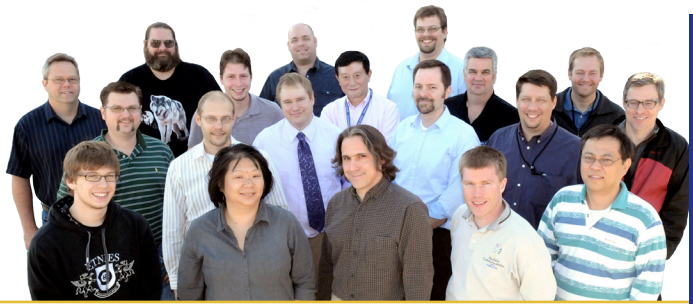
ALCF catalysts, performance engineers, and data analytics and visualization teams provide users with in-depth expertise and assistance in using ALCF computer systems. They help them achieve the best performance in their applications. The staff establishes strategic collaborations with the ALCF's project partners to maximize the benefits from using ALCF resources.

Performance Engineering Team

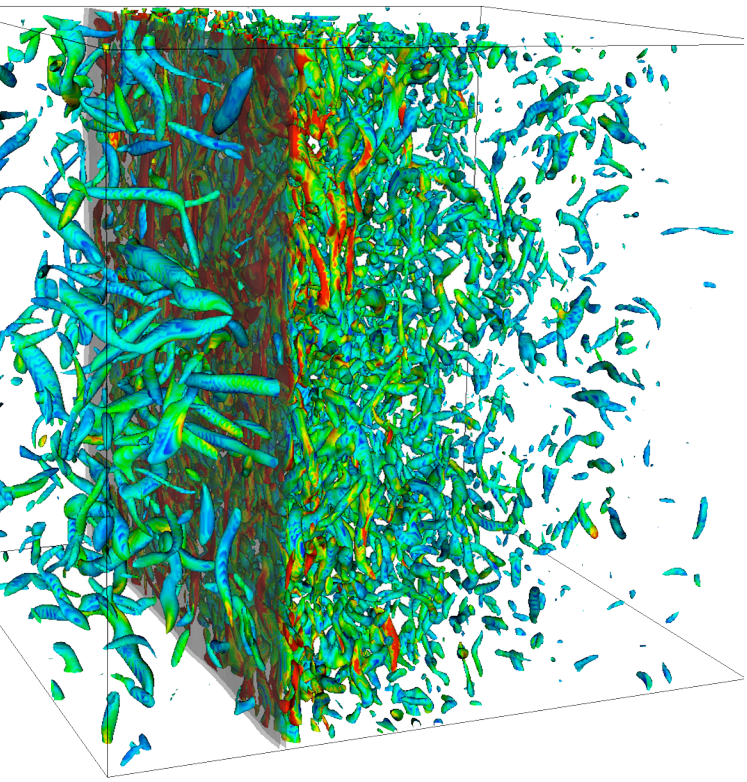
Catalyst Team

User Services and Outreach Team

Data Analytics and Visualization Team



Operations Team



In a fundamental study of shock/turbulence interaction, turbulent eddies are amplified upon passing through a shock wave.

Advancing Science with Powerful Resources

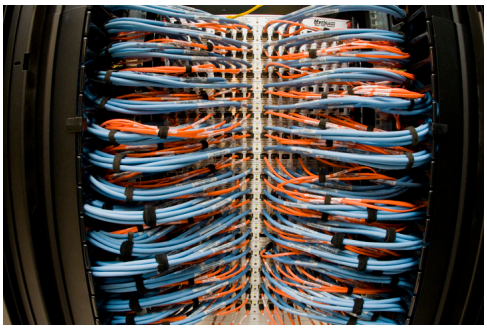
The ALCF is home to the IBM Blue Gene/P Intrepid, one of the fastest supercomputers in the world for open science. Intrepid features 40,960 quad-core compute nodes (163,840 processors) and 80 terabytes of memory. Intrepid boasts a peak performance of 557 teraflops, solidifying the ALCF's position as a leadership-class center for computation-driven scientific discovery. Despite its power, the energy-efficient system uses about one-third as much electricity as a machine of comparable size built with more conventional parts. In recognition of its significant energy savings, Argonne was awarded the HPCwire's Readers' Choice Award for Best Application of Green Computing at the annual Supercomputing Conference (SC09), held November 14-20, 2009 in Portland, OR.

The 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.

Breakthrough research under way at the Argonne Leadership Computing Facility delves into applied mathematics, climate research, combustion, nuclear physics, computer science, and other scientific disciplines.

Other ALCF resources include:

Networking



The Blue Gene/P uses five different networks for different communication operations. The 3-D torus network is used for general-purpose, point-to-point message passing as well as for collective operations using irregular communication or large message sizes. Each node has six nearest neighbors. Each link provides a bandwidth of 425 MB/s per direction, for a total bidirectional bandwidth of 5.1 GB/s. Though each node has six bidirectional links on each node, there is only one shared DMA engine. The 3-D torus network is also usable as a 3-D mesh.

The supercomputer connects to other research institutions using a total of 30 Gb/s of public network connectivity. This allows scientists to transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and the Metropolitan Research and Education Network (MREN).

Data Storage

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.

Current tape capacity installed and available is 6,500 tapes at 800 GB raw, in a 10,000-slot library. A second 10,000-slot library and 9,500 tapes are expected to enter production in early 2010.

Eureka

- Visualization and data analytics to transform data into useful knowledge
- 100 compute nodes: Each with (2) 2.0 GHz quad-core Xeon servers with 32 GB RAM
- 200 NVIDIA Quadro FX5600 GPUs in 50 S4s
- Memory: More than 3.2 terabytes of RAM
- Peak Performance: More than 111 mostly single precision teraflops of computation use a fraction of electricity compared to alternative architectures.

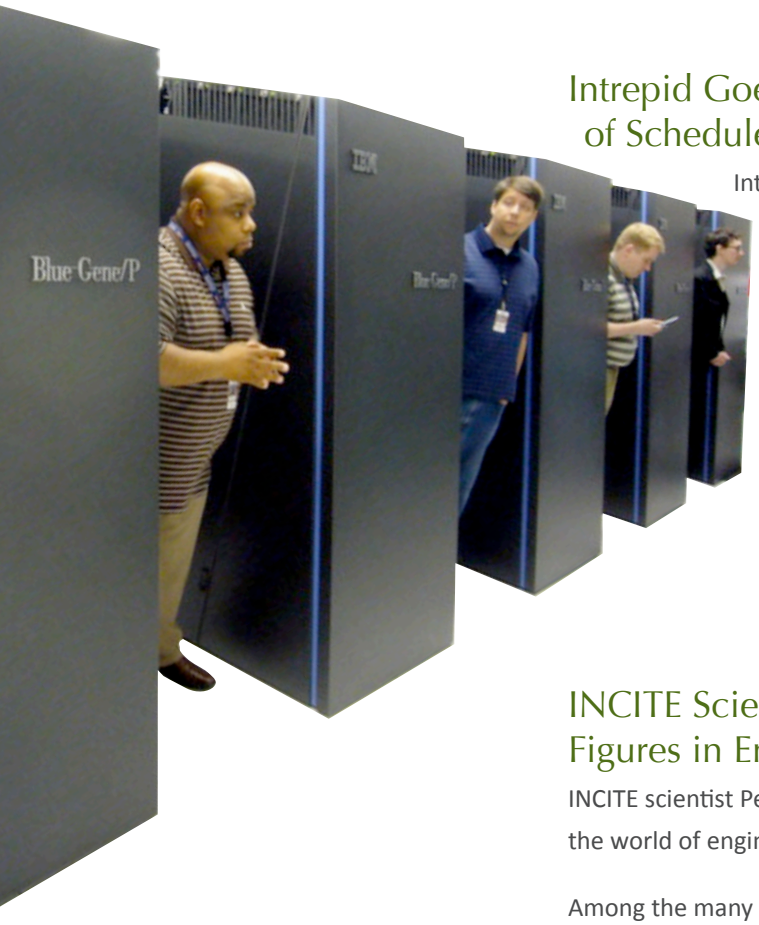
Gadzooks

- Test and development for visualization
- 4 compute nodes: Each with (2) 2.0 GHz quad-core Xeon servers with 32 GB RAM
- 8 NVIDIA Quadro FX5600 GPUs in 2 S4s

Flash simulation of a one-to-one mass ratio galaxy cluster merger with an impact offset computed on Argonne Leadership Computing Facility's Eure.

PI: Donald Q. Lamb
The University of Chicago

HIGHLIGHTS



Intrepid Goes into Full Production Five Months Ahead of Schedule

Intrepid, a 40-rack IBM Blue Gene/P system at the Argonne Leadership Computing Facility (ALCF) went into full production on February 2, five months ahead of schedule. Intrepid has 40,960 quad-core compute nodes (163,840 cores) and 80 terabytes of memory. Its peak performance is 557 teraflops. As a result, the ALCF nearly doubled the days of production computing available to the DOE Office of Science, INCITE awardees, and Argonne projects.

INCITE Scientist Named One of Top 25 Most Influential Figures in Engineering & Technology

INCITE scientist Peter Coveney was named one of the 25 most influential figures in the world of engineering and technology by Engineering & Technology magazine.

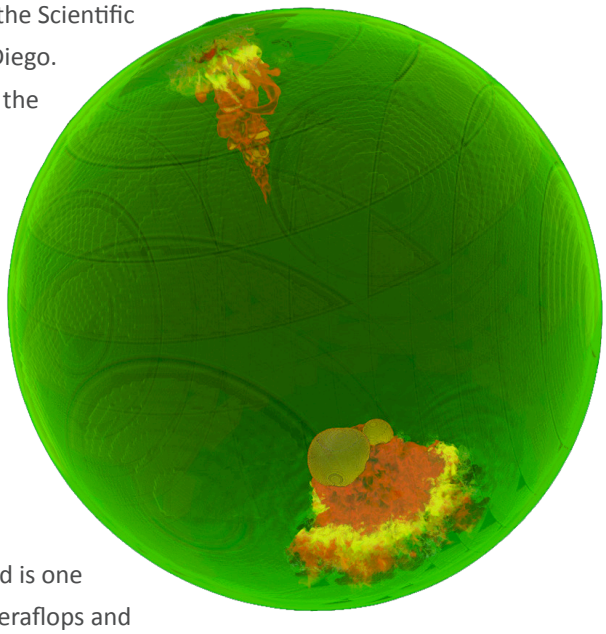
Among the many distinguished hats that Professor Peter Coveney dons for his work at University College London is director of the Centre for Computational Science.

At the ALCF, using computer simulations on the Blue Gene/P supercomputer, Professor Coveney leads a team of scientists and clinicians who conduct virtual experiments to study cerebral blood flow at the individual patient level. Their experiments include devising customized patient blood-flow simulations.

Having a computational tool that surgeons can use to examine the pressure and velocity variations in a patient's blood vessels and to predict what changes might occur as a result of interventional surgery will add immeasurably to a surgeon's "tool kit." Because patient-specific data is used as the basis of the simulation, treatments can be assessed for their effectiveness in the individual patient even before being administered, thus reducing risk and expense.
(For more details, see article on page 38).

Argonne Receives Two OASCR Awards at SciDAC 2009

Argonne received two of the U.S. Department of Energy's (DOE) Office of Advanced Scientific Computing Research (OASCR) Awards for visualizations, presented during the Scientific Discovery through Advanced Computing (SciDAC) conference held in San Diego. The top 10 winners were selected by the participants of the conference at the Electronic Visualization and Poster Night, held June 15.



The Argonne winning visualizations were "Turbulent Flow of Coolant in an Advanced Nuclear Reactor" and "Simulation of the Gravitationally Confined Detonation (GCD) Model of a Type Ia Supernovae for Ignition at Multiple Points."

Both the visualizations and the computer runs for the winning entries were done at the ALCF. The computations were carried out on one of the world's fastest and most energy-efficient supercomputers—Intrepid, Argonne's IBM Blue Gene/P. The visualizations were performed on Eureka with software developed at Argonne. Eureka is also located at the ALCF and is one of the world's largest graphics processing units, providing more than 111 teraflops and over 3.2 terabytes of RAM.

ALCF Staff Moves into the New Theory & Computing Sciences Building

ALCF staffed moved into a spacious, new Theory & Computing Sciences (TCS) building located at Argonne in September. Construction of the more than 200,000 square-foot, seven-story-tall TCS building was completed in late summer 2009. It features a unique zen garden and a vast library, as well as a multitude of open spaces and conference rooms.

IBM Blue Gene Series Awarded Medal of Technology and Innovation

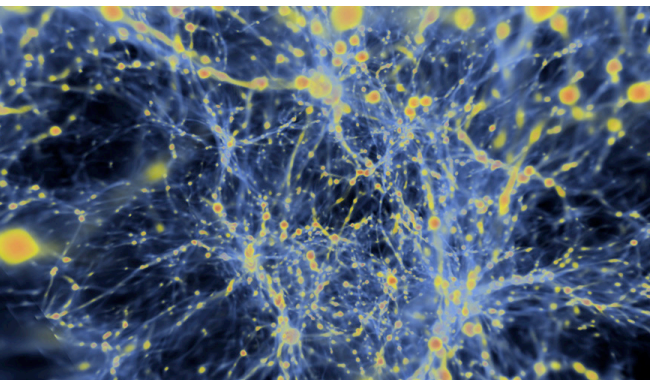
IBM Blue Gene Supercomputer recipient of the 2008 National Medal of Technology and Innovation

The IBM Blue Gene series of energy-efficient supercomputers, central to breakthrough scientific research around the world, was singled out by President Barack Obama as a Medal of Technology and Innovation award-winner on October 7 in Washington, D.C.

The U.S. Department of Energy, which leads the world in providing supercomputers for scientific research, began a R&D partnership with IBM in 2001 to develop the Blue Gene platform. Argonne, together with Lawrence Livermore National Laboratory (LLNL), worked on key aspects of the design and provided critical software components to ensure it was well suited to solve challenges in energy, the environment and national security. The ALCF is home to the 557-teraflops IBM Blue Gene/P supercomputer known as Intrepid, which is used for scientific and engineering computing. The Blue Gene/P features 40,960 quad-core compute nodes (163,840 processors) and 80 terabytes of memory. Peak performance is 557 teraflops.

The Medal of Technology and Innovation is described as the highest honor for technological achievement for outstanding contributions related to the nation's competiveness, standard of living, and quality of life through the development and commercialization of technological products. President Obama presented the medal to IBM, as well as four inventors who were also recognized for the award, at a White House ceremony on October 7. The medal program is administered by the United States Patent and Trademark Office and is awarded annually to individuals, teams and companies.

ALCF Prepares for Next-Generation Machine



In 2009, the ALCF obtained CD-3 approval for its next-generation machine, the contract was signed for the 10-petaflops system (with an option for an upgrade to a 20-petaflops system), and staff began to prepare for the new hardware.

Come 2012, the ALCF will be home to this supercomputer, which will give scientists a new tool for scientific discovery. It will be used for a wide range of research, including designing ultra-efficient electric car batteries, predicting fluid flow and convective heat transport in advanced nuclear reactor designs, understanding global climate change, improving combustion efficiency, and exploring the evolution of our universe.

DOE's Magellan Project Initiated to Explore Scientific Cloud Computing at ANL, LBNL

A new cloud project funded by the American Recovery and Reinvestment Act through the U.S. Department of Energy (DOE) was established to examine cloud computing as a potential new computing paradigm for scientists to accelerate discoveries in a variety of disciplines. The project will explore which science application programming models work well within the cloud, as well as evaluating the challenges that come with this new computing paradigm. Since the project is exploratory, it's been named Magellan in honor of the Portuguese explorer who led the first effort to sail around the globe and for whom the "clouds of Magellan" — two small galaxies in the southern sky — were named.

To test cloud computing for scientific capability, DOE centers at the Argonne Leadership Computing Facility (ALCF) in Illinois and the National Energy Research Scientific Computing Center (NERSC) in California installed similar computing hardware to what is found in most high performance computing clusters. In addition, each site is installing different storage hardware and environments. The combined set of systems create a cloud testbed that scientists can use for their computations while also testing the effectiveness of cloud computing for their particular research problems. The NERSC and ALCF facilities will be linked by a groundbreaking 100 gigabit-per-second network, developed by DOE's ESnet (another DOE initiative funded by the Recovery Act). Such high bandwidth will facilitate rapid transfer of data between geographically dispersed clouds and enable scientists to use available computing resources regardless of location.

Software Advancements Allow Data Interaction in Real-Time

To illustrate the importance—and feasibility—of visualization at a distance, scientists from several organizations, including institutions from both the National Science Foundation's TeraGrid project and the U.S. Department of Energy (DOE), teamed up to create a live demonstration. Images were streamed live at 10 gigabits per second from Eureka, one of the world's largest graphics supercomputers, which features 200 high-end graphics processing units in the ALCF, over DOE's ESnet, a high-speed network with dedicated bandwidth for moving large datasets worldwide, to an OptiPortal tiled display in the San Diego Supercomputer Center's booth at SC09. Eureka enables software such as vl3, a volume rendering toolkit developed at Argonne and the University of Chicago, that leverages graphics hardware to visualize such data sets in real time.

The simulation was done as part of a 2009 TeraGrid resource allocation entitled "Projects in Astrophysical and Cosmological Structure Formation," designed to simulate the cosmic structures of the early universe by calculating the gravitational clumping of intergalactic gas and dark matter. The model uses a computational grid made up of 40,003 cells; contained 64 billion dark matter particles; and took more than four million CPU hours to complete.

ASCR-Funded Computers Take Top Honors at SC09 HPC Challenges

Results of the "Best Performance" awards, which measure excellence in handling computing workloads, were announced at SC09 and included ASCR-funded supercomputers. Oak Ridge Leadership Computing Facilities' (OLCF) Jaguar took three first place awards for HPL code (solving a dense matrix of linear algebra equations), STREAM (measures how fast a node can retrieve and store information), and executing the Fast Fourier Transformation (FFT). For running the RandomAccess measure of the rate of integer updates to random locations in a large global memory array, the IBM Blue Gene machine at LLNL took first, the Blue Gene/P at the ALCF took second, and the Jaguar at OLCF took third place.

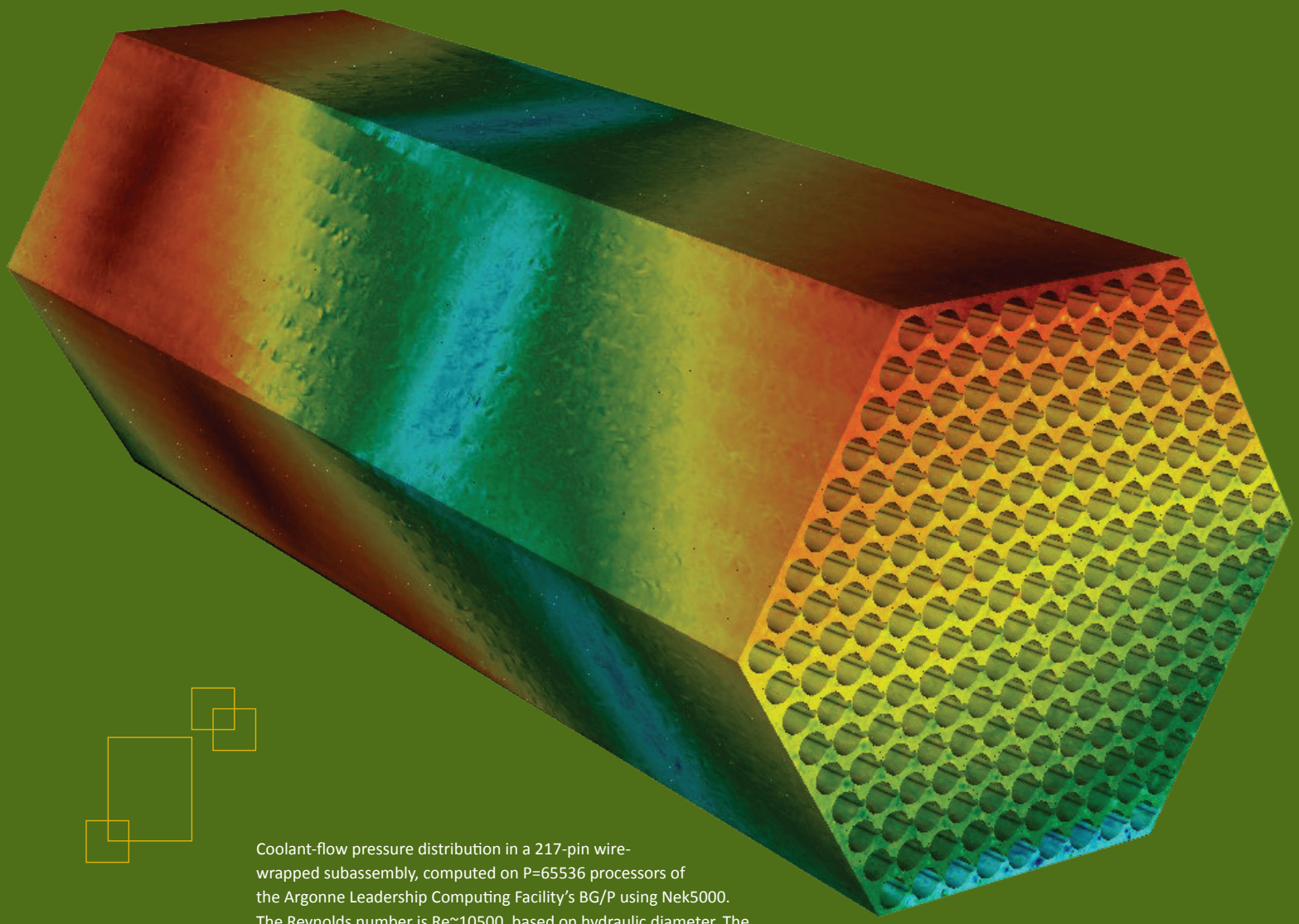
ANL's Green Computing Wins 2009 HPCwire Readers' Choice Awards

Argonne National Laboratory was awarded the HPCwire's Readers' Choice Award for Best Application of Green Computing. The award was presented by Tomas Tabor, publisher of HPCwire, at SC09, the annual supercomputing conference held Nov. 14-20 in Portland, Ore. The annual HPCwire Readers' and Editors' Choice Awards are determined through a survey conducted by HPCwire, online polling of the global HPCwire audience, along with a rigorous selection process involving HPCwire editors and industry luminaries.

Argonne compute and storage systems have "smart power" management functionality that allows them to turn off or throttle back the power consumption. The Argonne Leadership Computing Facility (ALCF) is home to Intrepid, an energy-efficient IBM Blue Gene/P supercomputer, which uses about one-third as much electricity as a comparable supercomputer. The ALCF achieves savings in energy through a variety of innovative operational techniques, including methods employed to cool the supercomputer – a process that normally requires more electricity than powering the machine itself. In addition, the ALCF works with IBM to use the warmest possible water temperature necessary to effectively cool the computer systems, leading to even greater savings and reduced environmental impact.

Argonne's Cloud Computing Efforts Featured on "Chicago Tonight" News Program

Rich Samuels, a news correspondent with the "Chicago Tonight" news program on WTTW-Channel 11, visited Argonne National Laboratory for a segment on cloud computing. "Cloud computing" is a model for on-demand access to computing resources – networks, servers, and software – that can be easily provisioned as needed over the Internet. The concept's most visible adoption is in the commercial world, but Dr. Kate Keahey, a computer scientist in the Mathematics and Computer Science Division at Argonne, has been promoting its use in a far different area: science. Keahey designed and developed the "workspace service" software that enables users to deploy virtual machines on remote resources. This work was followed by tools enabling users to deploy virtual clusters sharing configuration and security context. These tools form the open source Nimbus toolkit, which other researchers have extended to explore such questions as data privacy and storage management in the clouds. Keahey and Argonne's Ian Foster were interviewed in the news report, which was part of the 7 p.m. broadcast on Nov. 10.



Coolant-flow pressure distribution in a 217-pin wire-wrapped subassembly, computed on P=65536 processors of the Argonne Leadership Computing Facility's BG/P using Nek5000. The Reynolds number is Re~10500, based on hydraulic diameter. The mesh consists of 2.95 million spectral elements of order N=7 (~988 million gridpoints). The simulation pictured is a watershed computation, as it is the first to exceed one million elements (2.95 M used) and the first to use one billion gridpoints (0.988 B used). This simulation was performed using the Nek5000 code employing 68826 spectral elements of order N=7 and run on 8192 core of the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory.

PI: Paul Fischer
Argonne National Laboratory

RESEARCH DISCOVERIES

Solving Pressing National Challenges through 2009 INCITE Projects

In 2009, DOE allocated 400 million hours of computing time to the following 28 research projects (18 renewals, 10 new) at the ALCF through its INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. INCITE supports computationally intensive, large-scale research projects that address pressing scientific and national challenges.

Applied Mathematics

- Reactor Core Hydrodynamics
  Paul Fischer, Argonne National Laboratory
  Intrepid Allocation: 30 Million Hours

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
  Intrepid Allocation: 70 Million Hours

Biological Sciences

- Computational Protein Structure Prediction and Protein Design
  David Baker, University of Washington
  Intrepid Allocation: 12 Million Hours
- Gating Mechanism of Membrane Proteins
  Benoit Roux, Argonne National Laboratory and The University of Chicago
  Intrepid Allocation: 30 Million Hours
- Large-Scale Simulations of Cardiac Electrical Activity
  Jeffrey Fox, Cornell University
  Intrepid Allocation: 21,405,500 Hours
- Sculpting Biological Membranes by Proteins
  Klaus Schulten, University of Illinois
  Intrepid Allocation: 9.24 Million Hours
- 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
  Intrepid Allocation: 3 Million Hours

Chemical Sciences

- Molecular Simulation of Complex Chemical Systems
  Christopher Mundy, Pacific Northwest National Laboratory
  Intrepid Allocation: 2 Million Hours
- Molecular Simulations of Surfactant-Assisted Aqueous Foam Formations
  Kelly Anderson, Procter and Gamble
  Intrepid Allocation: 6 Million Hours
- Water in Confined States
  Giulia Galli, University of California–Davis
  Intrepid Allocation: 2 Million Hours

Climate Research

- Climate-Science Computational End Station Development and Grand Challenge Team
  Warren Washington, National Center for Atmospheric Research
  Intrepid Allocation: 7.5 Million Hours
- Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence
  Susan Kurien, Los Alamos National Laboratory
  Intrepid Allocation: 25 Million Hours
- The Role of Eddies in the Meridional Overturning Circulation
  Paola Cessi, Scripps Institution of Oceanography/University of California–San Diego
  Intrepid Allocation: 5 Million Hours

Combustion

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

Computer Science

- Blue Gene/P Plan 9 Measurements on Large-Scale Systems
  Ronald Minnich, Sandia National Laboratories
  Intrepid Allocation: 8 Million Hours
- Performance Evaluation and Analysis Consortium End Station
  Patrick Worley, Oak Ridge National Laboratory
  Intrepid Allocation: 8 Million Hours

- **Engineering**
  - Fundamental Study of Shock/Turbulence Interaction
    Sanjiva Lele, Stanford University
    Intrepid Allocation: 8 Million Hours
  - Petascale Adaptive CFD for Anisotropic Flows
    Kenneth Jansen, Rensselaer Polytechnic Institute
    Intrepid Allocation: 5 Million Hours
- **Environmental Sciences**
  - Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz
    Thomas Jordan, Southern California Earthquake Center
    Intrepid Allocation: 5 Million Hours
- **Lattice Gauge Theory**
  - Lattice QCD
    Paul Mackenzie, Fermi National Accelerator Laboratory
    Intrepid Allocation: 67 Million Hours
- **Materials Sciences**
  - Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles
    Christopher Wolverton, Northwestern University
    Intrepid Allocation: 1 Million Hours
  - Large-Scale Condensed Matter and Fluid Dynamics Simulations
    Peter Coveney, University College London
    Intrepid Allocation: 40 Million Hours
  - Linear Scale Electronic Structure Calculations for Nanostructures
    Lin-Wang Wang, Lawrence Berkeley National Laboratory
    Intrepid Allocation: 1 Million Hours
  - Modeling the Rheological Properties of Concrete
    William George, National Institute of Standards and Technology
    Intrepid Allocation: 750,000 Hours
- **Nuclear Energy**
  - Predictions of Thermal Striping in Sodium–Cooled Reactors
    Andrew Siegel, Argonne National Laboratory
    Intrepid Allocation: 7.5 Million Hours
- **Nuclear Physics**
  - Computational Nuclear Structure
    David Dean, Oak Ridge National Laboratory
    Intrepid Allocation: 10 Million Hours
- **Plasma Physics**
  - High-Resolution Global Simulation of Plasma Microturbulence
    William Tang, Princeton Plasma Physics Laboratory
    Intrepid Allocation: 6 Million Hours
  - Three-Dimensional Particle-in-Cell Simulations of Fast Ignition
    Chuang Ren, University of Rochester
    Intrepid Allocation: 1.5 Million Hours

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.

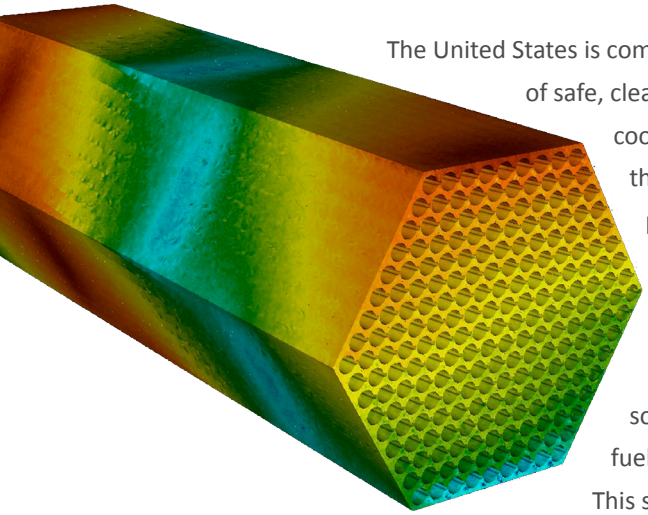
The INCITE program encourages proposals from industry, universities, and research institutions. Proposals are peer-reviewed and chosen solely on the basis of scientific merit and readiness to use the LCF computers at scale. More information about the program can be found on DOE's Office of Science website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

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Applied Mathematics

Reactor Core Hydrodynamics

PI: Paul Fischer, Argonne National Laboratory
Intrepid Allocation: 30 Million Hours



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 demand. Liquid-metal-cooled fast reactors are a key component of this strategy in that they permit the recycling of nuclear fuel and are expected to be an economical source of power.

A research team led by Paul Fischer of Argonne National Laboratory and including 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. This simplified geometry allows them to resolve all turbulent motion with no modeling assumptions.

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. Validated Nek5000 results are being used to benchmark steady-state Navier-Stokes codes that employ turbulence models and to provide input to reactor design codes that require only coarse (mean flow) data. Visualization support for the project is provided by the VisIt group at Lawrence Livermore National Laboratory.

Future 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

Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernovae Models

PI: Donald Lamb, NNSA ASC/Alliance Flash Center,
The University of Chicago
Intrepid Allocation: 70 Million Hours

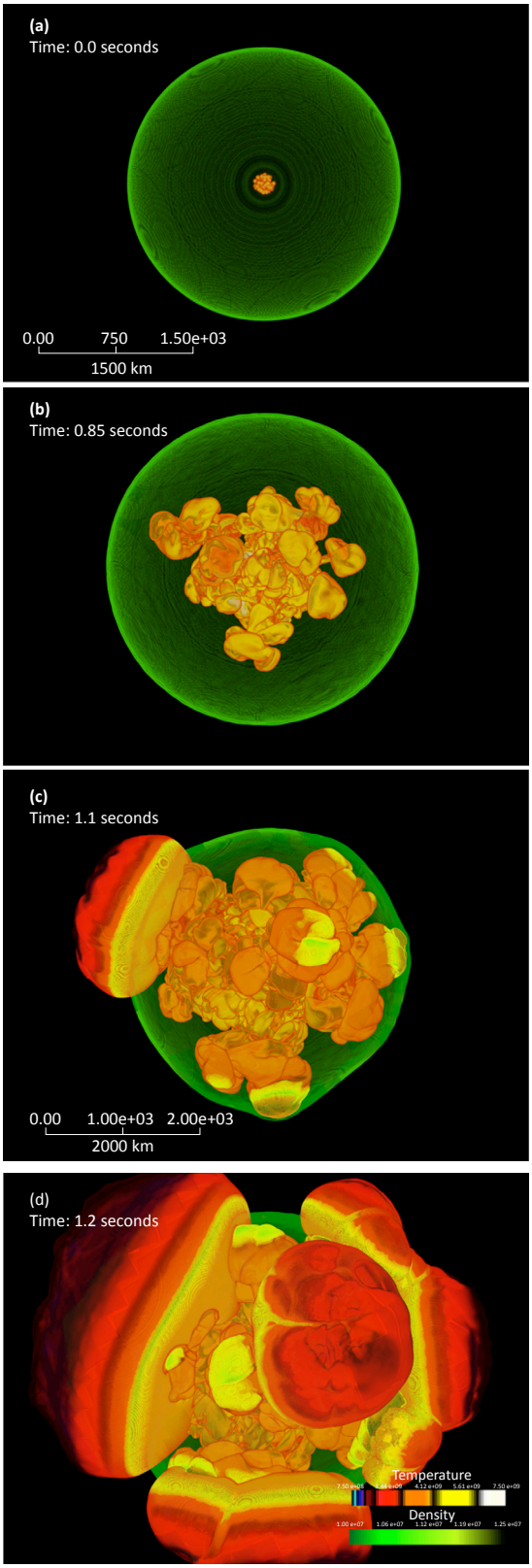
Led by Donald Lamb of the University of Chicago's NNSA ASC/Alliance Flash Center, researchers studied critical aspects of Type Ia supernovae, some of the brightest, most powerful exploding stars in the universe. These supernovae are responsible for creating many of the elements from which we are made and are important for measuring distances in the universe.

Two major challenges currently face scientists in understanding these stars: 1) buoyancy-driven turbulent nuclear burning, a key physical process in the star, is not fully understood, and 2) few simulations of the four current models of the star have been done.

Working together, 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, then ran a grid of simulations for different physical conditions. Researchers also developed the parallel processing tools needed to analyze the large amounts of data produced by the simulations.

To date, the team has simulated all current models of Type Ia supernovae on the Blue Gene/P. These simulations led to the discovery of robust signatures for the different supernova models, holding out the promise that observations can discriminate among them. Their work represents the first comprehensive, systematic validation of current models of Type Ia supernovae.

The team also has simulated buoyancy-driven turbulent nuclear combustion. A preliminary analysis of their results showed that the flame surface is complex at large scales and smooth at small scales, suggesting that the burning rate may be determined by the properties of the flame at large scales. Their findings 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.

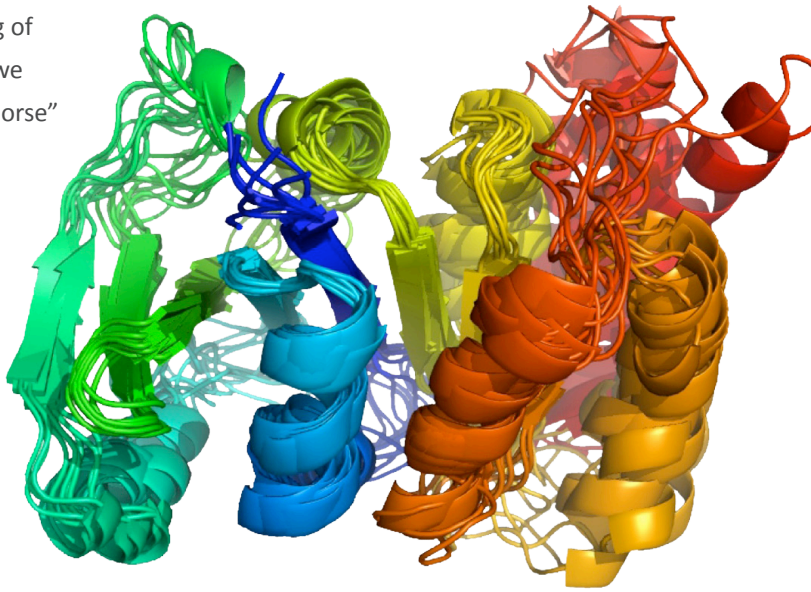


Biological Sciences

Computational Protein Structure Prediction and Protein Design

PI: David Baker, University of Washington
Intrepid Allocation: 12 Million Hours

To achieve a more complete understanding of biological systems and how they operate, we must first understand proteins, the "workhorse" molecules of all living things. Scientists' conventional method of identifying protein structure—nuclear magnetic resonance (NMR)—is expensive and time-consuming. In addition, using NMR to analyze larger proteins relies on deuteration—that is, the incorporation of the stable isotope deuterium—and carries with it the risk of losing significant information about the protein's side-chain proton-proton distances.



A team led by David Baker of the University of Washington is using the Blue Gene/P supercomputer at ALCF to focus on three areas of inquiry: 1) computing protein structures from limited experimental data; 2) designing proteins to bind tightly to specific regions on a target; and 3) designing new enzyme catalysts. Using these resources, the team developed an iterative protocol that enabled them to increase the size range of accessible protein structures compared to the conventional Rosetta protocol. Their newly designed method allowed them to determine the structure of proteins in over 200 amino acids—a potentially significant breakthrough.

The team has also designed proteins that bind with and neutralize viruses, and catalysts for hydrogen production, solar capture, and other energy-related applications.

Biological Sciences

Gating Mechanisms of Membrane Proteins

PI: Benoit Roux, Argonne National Laboratory and The University of Chicago
Intrepid Allocation: 30 Million Hours

In living organisms, proteins control many biological processes in the cell membrane, ranging from the production of biofuels to cleaning up toxic organic waste. Large-scale gating motions that occur at a relatively slow pace 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. When those channels malfunction, they can lead to cardiac arrhythmia and neurological abnormalities.

Benoit Roux, from Argonne National Laboratory and the University of Chicago, in collaboration with researchers from the University of Illinois at Urbana-Champaign, used high-performance computing on the Blue Gene/P supercomputer at the ALCF to break new ground in understanding how these membrane proteins work.

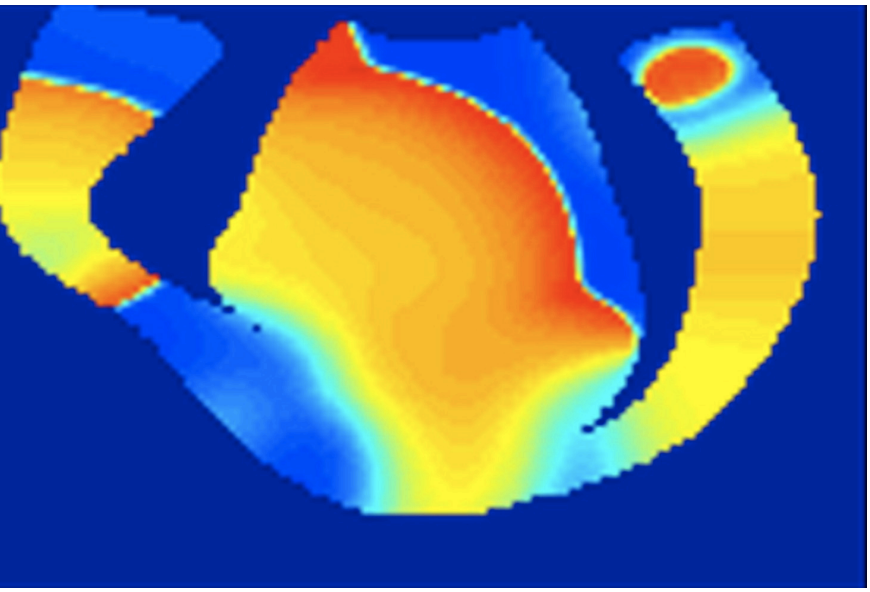
Exploiting state-of-the art developments in molecular dynamics and protein modeling, the team constructed models of voltage-gated potassium channels—the most realistic representations of these channels obtained to date—and ran simulations on the Blue Gene/P. Their calculations helped scientists understand how the gating movement works. Their research revealed that the electric field responsible for voltage activation was indeed more intense than at other equivalent positions across the membrane far away from the protein.

The findings signal the possibility of better-designed therapeutic drugs as well as the construction of artificial biomemetic nano-switches. The team's work is expected to set the standard for further inquiry in this important area.

Biological Sciences

Large-Scale Simulations of Cardiac Electrical Activity

PI: Jeffrey Fox, Cornell University
Intrepid Allocation: 21,405,500 Hours



Catastrophic rhythm disturbances of the heart are a leading cause of death in the United States. Treatment and prevention of cardiac rhythm disorders remain difficult because the electrical signal that controls the heart's rhythm is determined by complex, multi-scale biological processes. However, recent advances in experimental technologies have allowed for more detailed characterizations of normal and abnormal cardiac electrical activity.

In work funded by the National Institutes of Health (NIH), researchers are using U.S. Department of Energy INCITE allocations on the ALCF's Blue Gene/P to rapidly test hypotheses for the initiation and maintenance of rhythm disorders. These large-scale computer simulations represent 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.

The results of these simulations may help elucidate mechanisms of heart rhythm disorders that pose a significant health risk to the general public. An improved understanding of these disorders will help lead to safer and better treatments for patients.

Certain activation sequences have been shown to be particularly effective at inducing arrhythmias in canine experimental models. Researchers plan to study these sequences in large-scale simulations of the canine heart to identify the mechanism by which wave break and the induction of an arrhythmia might occur.

Biological Sciences

Sculpting Biological Membranes by Proteins

PI: Klaus Schulten, University of Illinois, Urbana-Champaign
Intrepid Allocation: 9.24 Million Hours

Inside the cells that make up the human body are many organelles—that is, differentiated structures responsible for carrying out a specific cell function, such as growth, division, and movement. The organelles themselves are intricately curved internal membranes.

Biologists have discovered that during the life of the cell, proteins—some of the smallest of the cell's components—work to "sculpt" the cell's membrane into these specific shapes. Rarely do membranes form these shapes spontaneously; instead, they interact with proteins to generate the required shape.

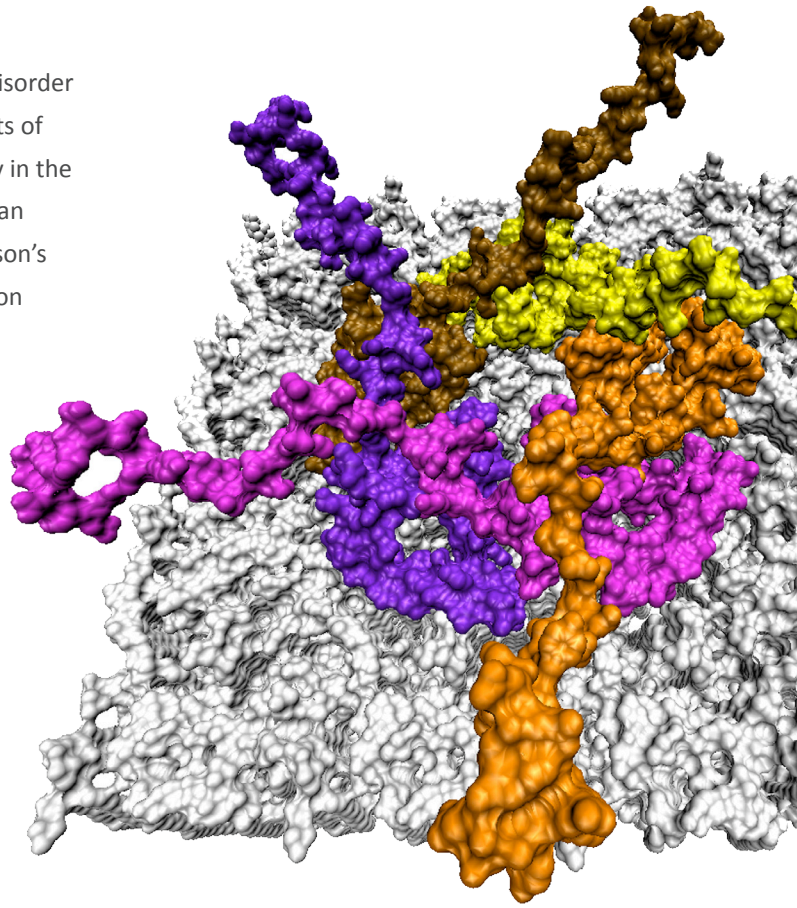
Scientists have found that proteins do this sculpting both inside and outside the cell membrane. How proteins create these curves is one of the most fascinating areas in modern cell biology and the subject of much recent study.

Researchers under the direction of Klaus Schulten, University of Illinois at Urbana-Champaign are using the Blue Gene/P supercomputer at the ALCF to get a closer look at the work of proteins inside a cell. The Blue Gene/P serves as a kind of computational "microscope" that enables the team to identify molecular building blocks and the shapes resulting from various proteins. Simulations created on the Blue Gene/P have enabled the team to observe and describe certain aspects of the proteins' behavior. Their findings provide a first-ever look at how proteins work in concert to form cellular structures.

Biological Sciences

Simulation and Modeling of Membrane Interactions with Unstructured Proteins and Computational Designs of Membrane Channels for Absorption of Specified Ions

PI: Igor Tsigelny, University of California—San Diego
Intrepid Allocation: 3 Million Hours



As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Currently in the United States, the condition affects more than 2 million people. In economic terms, Parkinson's disease exacts an annual cost of $25 billion on the U.S. economy alone.

Scientists from the University of California, San Diego, under the direction of Igor Tsigelny at the UCSD's San Diego Supercomputer Center, have shown that the aggregation of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes.

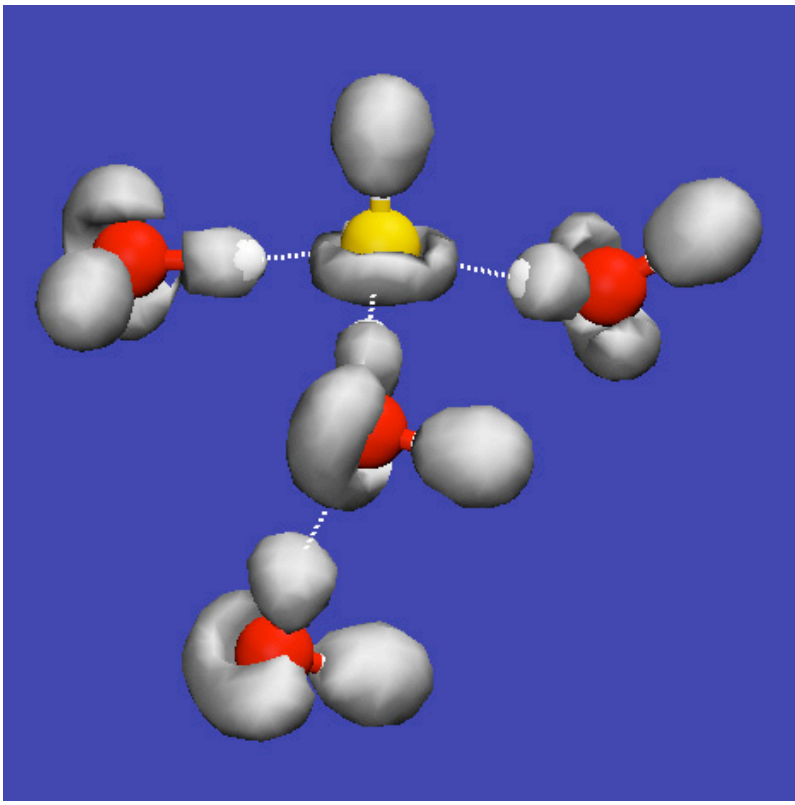
Researchers are leveraging the high-end computation power of the Blue Gene/P at the Argonne Leadership Computing Facility to learn more about the molecular basis of the disease and to explore ways to treat it. Their research is providing insights into the molecular mechanism for the progression of Parkinson's disease and will have broad applicability to other diseases. The findings also provide a test bed for identifying possible therapeutic interventions through computational modeling.

The correlations between the molecular dynamics modeling predictions and laboratory experimental results has been encouraging, and the team expects to make steady progress both with the computational model itself and with the design of effective drugs based on modeling and simulations. In the next phase, the team will focus on a more comprehensive investigation of alpha-synuclein penetration into the membrane, including a thorough study of pore creation. The scope of the team's work has increased in both the number and scale of simulations conducted.

Chemical Sciences

Molecular Simulation of Complex Chemical Systems

PI: Christopher Mundy, Pacific Northwest National Laboratory
Intrepid Allocation: 2 Million Hours



Understanding reactions on a molecular scale is critical to solving many of the challenges facing the 21st century. Yet, our knowledge about those reactions is still in its infancy. Leadership class computing provides computational molecular simulations of reactions that will lead scientists to unprecedented discovery, moving the field of molecular simulation to a radically new simulation protocol.

Led by Christopher Mundy, researchers at Pacific Northwest National Laboratory—collaborating with New York University, Lawrence Livermore National Laboratory, and the University of California, Irvine—created detailed models of chemical processes at interfaces by applying statistical mechanical sampling methods in conjunction with density functional theory (DFT)-based interaction potentials.

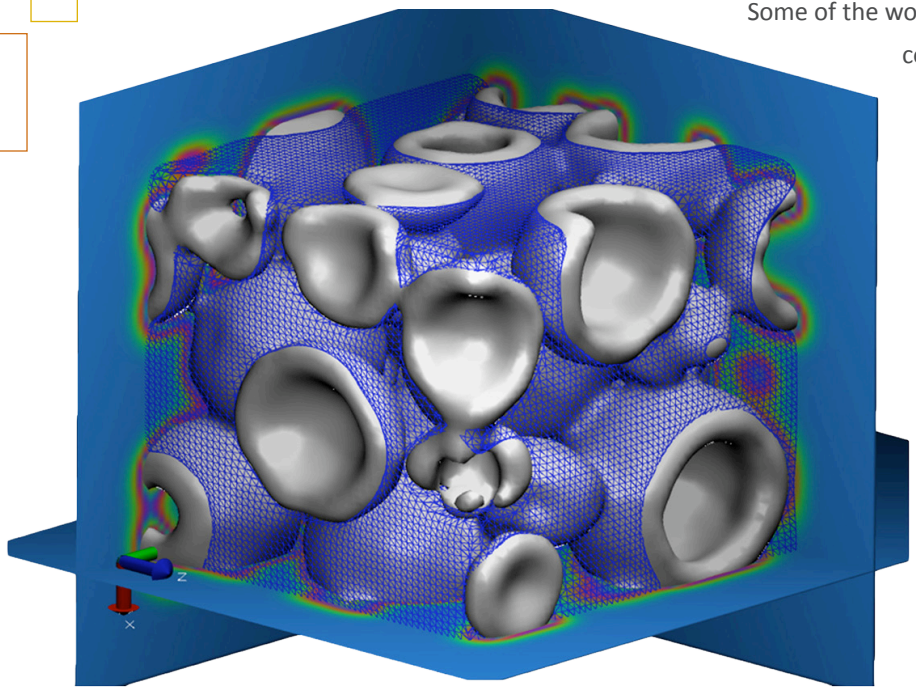
The basic chemical physics of these leadership calculations offer a detailed, molecular-scale picture of ions and reactions near interfaces. The researchers have obtained results on the free energies of transfer of OH- from the bulk to interface. Through the direct simultaneous sampling of different reactions' coordinates, a picture is emerging of how dramatically the structure and chemistry of species at interfaces differ from the bulk.

Specifically, their findings on OH- reveal a weak propensity for the hydroxide anion at the air-water interface, a prediction exactly opposite of what scientists had deduced from classical empirical potentials. This study reinforces the notion that novel chemistry can occur in the vicinity of the air-water interface—a far-reaching implication for scientists' understanding of chemical processes.

Chemical Sciences

Molecular Simulations of Surfactant-Assisted Aqueous Foam Formations

PI: Kelly Anderson, Procter and Gamble
Intrepid Allocation: 6 Million Hours



Some of the world's most well-known and highly regarded companies seek out Argonne's computing capability and technical expertise to convert that knowledge into transformative products and technologies. Procter & Gamble (P&G), a leading consumer products company and global marketer of dozens of brands, is among them.

Under the direction of Kelly Anderson, a research team from P&G uses the Blue Gene/P supercomputer at the ALCF to investigate the molecular mechanisms of bubble formation in foams. The team performs computer simulations at an unprecedented scale on the dissolving of soap and foaming of suds. Researchers have developed coarse-grained models for several foaming surfactants—that is, the wetting agents in cleaning products that break the surface tension of water so that the product can work. How well mixtures of surfactants and polymers work in water becomes a key performance driver for the formulations of many of P&G's household products.

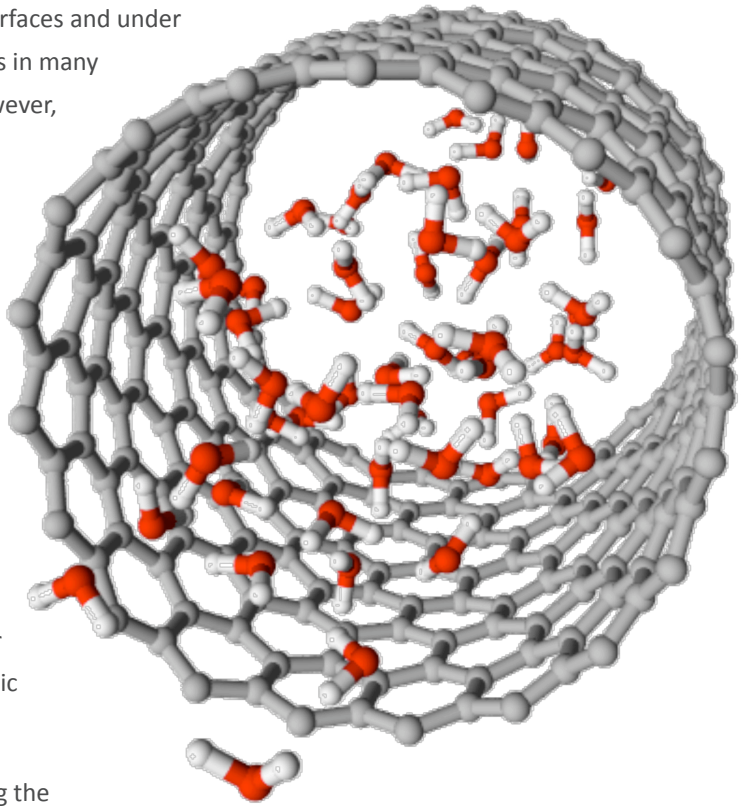
The team has published several papers on its findings to date. This research is expected to help escalate innovation at Procter & Gamble, bringing consumer products to market faster and more efficiently.

Chemical Sciences

Water in Confined States

PI: Giulia Galli, University of California—Davis
Intrepid Allocation: 2 Million Hours

Unraveling the properties of water at organic and inorganic interfaces and under pressure is key to understanding the behavior of other materials in many natural environments and how biological systems function. However, the challenge is compounded when water is compressed or confined in very small spaces, as it is on the surface of proteins, in channels that transport matter at the nanoscale, or in natural rocks.



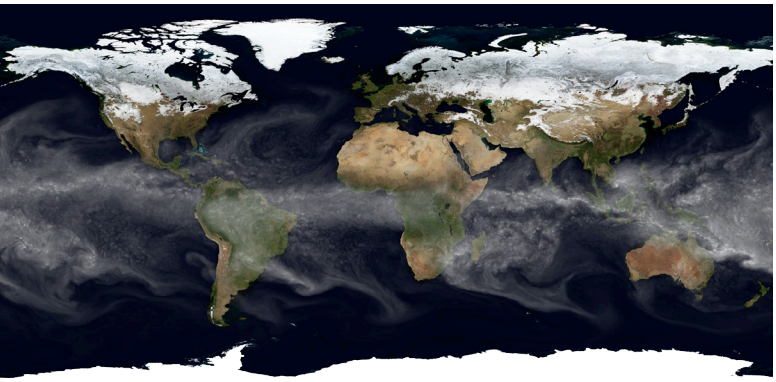
A team led by Giulia Galli of the University of California, Davis used the Blue Gene supercomputers at the ALCF and IBM Blue Gene Watson Research Laboratory to investigate water in confined states and under pressure. Researchers studied pure water under pressure and water in contact with graphite, nanotubes, hydrogenated diamond surfaces, and biocompatible materials such as silicon carbide. Their work to date has 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.

Researchers identified the key role electrons play in determining the arrangement of water molecules at both hydrophilic and non-polar surfaces. They computed vibrational spectra and provided predictions and interpretations of what should be seen experimentally when measuring how water molecules vibrate in contact with non-polar surfaces. They have applied the same techniques to determine the melting line of ice under pressure. Their findings can be applied to solve complex problems in biology and materials science.

Climate Research

Climate-Science Computational End Station Development and Grand Challenge Team

PI: Warren Washington, National Center for Atmospheric Research
Intrepid Allocation: 7.5 Million Hours



When human activity causes massive amounts of carbon dioxide and other greenhouse gases to be released into the earth's atmosphere, global warming occurs. Scientists are alarmed at the rate at which global temperatures are rising—far faster than any time known in geological history.

Using the Blue Gene/P supercomputer at the ALCF, a team led by Warren Washington and including researchers from the National Center for Atmospheric Research and the U.S. Department of Energy laboratories is performing advanced computation to develop complex, intricate climate models. The Climate Computational End Station (CCES) organizes and coordinates these and other computational efforts. CCES is helping to advance climate science through aggressive model development and an extensive suite of climate simulations. Dr. Washington's team tested a new, highly scalable method for solving the fluid dynamics of the atmosphere. Their findings will help scientists evaluate potential risks to the climate system and help governments formulate policy that curbs global warming and prevents further disruption to the planet's environment.

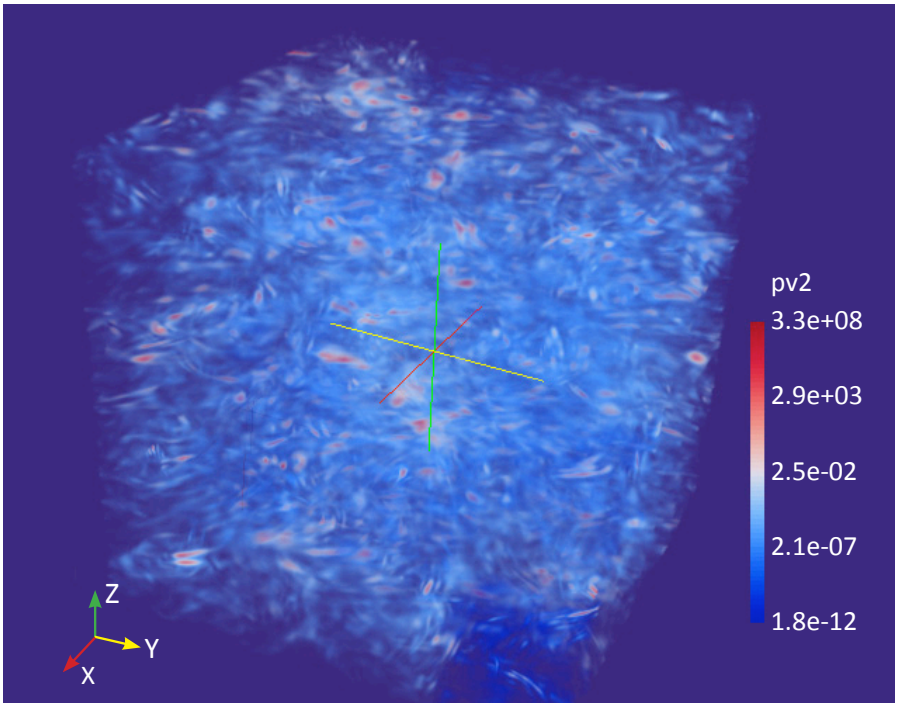
In the next phase of this project, researchers will use HOMME to perform standard climate model benchmark simulations for comparisons with other models. Their findings will help scientists evaluate potential risks to the climate system and help governments formulate policy that curbs global warming and prevents further disruption to the planet's environment.

Climate Research

Numerical Study of Multiscale Coupling in Low-Aspect, Ratio Rotating Stratified Turbulence

PI: Susan Kurien, Los Alamos National Laboratory
Intrepid Allocation: 25 Million Hours

What scientists learn from representative models is only as accurate as the models themselves. Accordingly, current climate models use approximations that are accurate over a large part of the ocean but lack the high resolution necessary for accuracy at a regional level—for example, in the Gulf of Mexico or the Arctic basin.



A research team led by Susan Kurien of Los Alamos National Laboratory performed extremely high-resolution simulations to quantify the behavior of rotating and stratified turbulent flows in which several time and spatial scales may be simultaneously important, and for which non-hydrostatic effects are not negligible and a statistical description becomes necessary.

Using the IBM Blue Gene/P supercomputer at the ALCF, researchers computed, analyzed, and visualized turbulence for various aspect ratio domains. The high-resolution simulations allowed the team to verify theoretical predictions about energy and potential enstrophy distribution in the small scales. Horizontal energy, for example, is organized into flat, disk-like structures, while the potential enstrophy in the same flow exhibits primarily a three-dimensional structure.

Performed over time, such simulations will reveal how small-scale turbulence affects the climate scales in both space and time, and may lay the groundwork for next-generation climate research.

Climate Research

The Role of Eddies in the Meridional Overturning Circulation

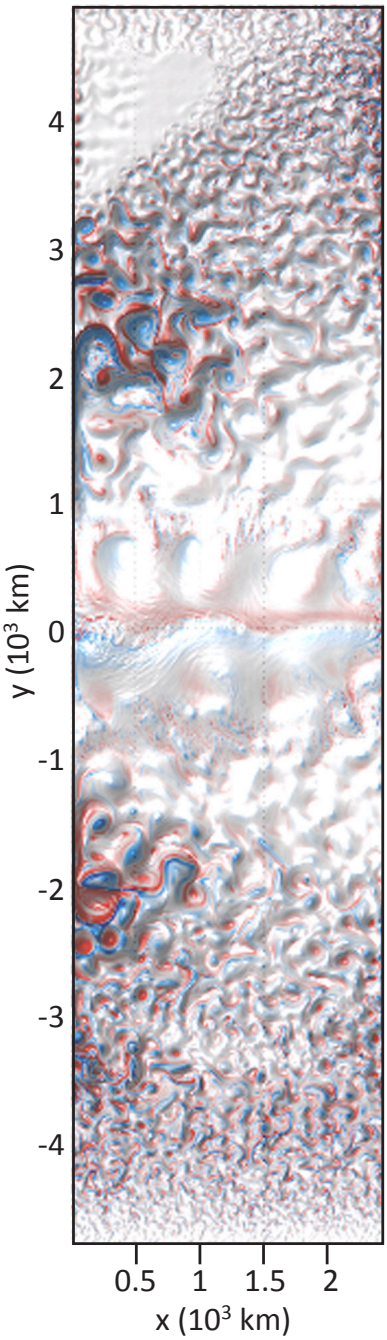
PI: Paola Cessi, Scripps Institution of Oceanography/University of California—San Diego
Intrepid Allocation: 5 Million Hours

Unlike the atmosphere, which is heated "internally" by the sun's radiation, the ocean is heated chiefly on its surface, with heat transferred from the surface to its depths in stratified temperature layers. Because we do not yet understand the processes that provide for the heat transfer or cause this stratification of temperatures, it is impossible to accurately predict climate scenarios.

Using the Blue Gene/P supercomputer at the ALCF, researchers led by Paola Cessi of the Scripps Institution of Oceanography at the University of California, San Diego, analyzed high-resolution models of the ocean that employed such variables as wind speed, surface temperature, and abyssal mixing.

To date, the research has yielded important findings. For example, the team discovered that eddies—vortices that shed off the ocean's main currents—play an essential role in setting the vertical profile of temperature in the ocean. Other findings revealed that the temperature distribution in the ocean's intermediate layers is set by the dynamics of the currents and eddies around Antarctica, and that this region is key to the strength of the Meridional Overturning Circulation (MOC). In addition, the team found that the effects of a thin coastal upwelling region can be represented by a set of effective boundary conditions that relate the longshore buoyancy gradient to eddy fluxes of buoyancy and potential vorticity away from the boundary.

The team's work has highlighted the importance of being able to create high-resolution simulations to study the ocean. It has also revealed the importance of the dynamics of the southern hemisphere's ocean on the MOC in the northern hemisphere (and, thus, its influence on the climate of Europe and North America).

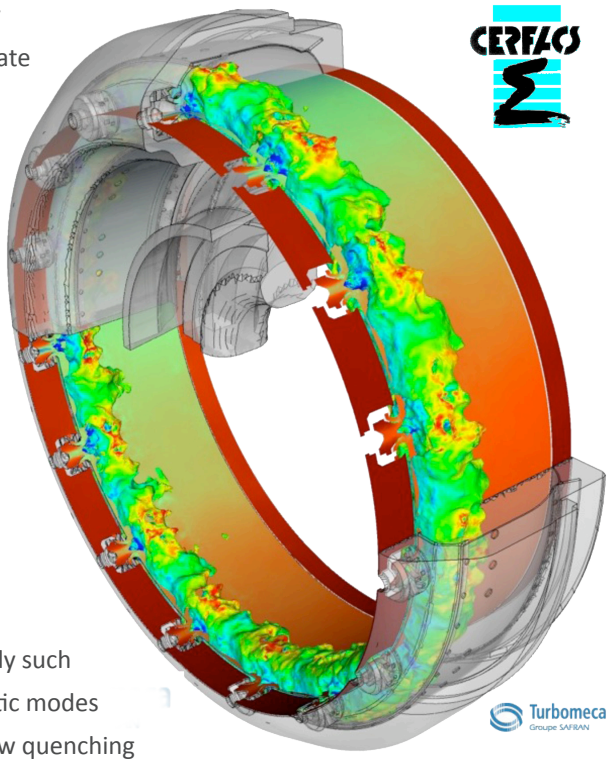


Combustion

Massively Parallel Simulation of Combustion in Gas Turbines

PI: Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Intrepid Allocation: 8 Million Hours

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 to simulate 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, re-ignition, 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 researchers to reproduce the behavior of a gas turbine demonstrator equipped with 15 burners and a new injector design. The LES singled out the presence of a thermo-acoustic instability that impacts the flow behavior. Their results reveal that, in this case, flame anchoring is not jeopardized by the instability. The study also allowed researchers to study such important physical mechanisms as burner interactions, azimuthal acoustic modes generation, flame propagation from one burner to its neighbors, and how quenching occurs.

The project's next phase—performing full-chamber LES—will involve top-of-the-edge modeling as well as such innovative computer science techniques as dynamic load balancing and conditional domain decomposition. The team's findings have real-world application in energy production (for example, in industrial gas turbines) and propulsion (as seen in helicopter and aircraft engines).

Computer Science

Blue Gene/P Plan 9 Measurements on Large-Scale Systems

PI: Ronald Minnich, Sandia National Laboratories
Intrepid Allocation: 8 Million Hours

A team of researchers led by Ronald G. Minnich of Sandia National Laboratories worked to provide a new software environment for the Blue Gene/P supercomputer at ALCF. Their work was aimed at making the supercomputer appear to be part of the user's desktop system rather than a remote, hard-to-access external computer.

The team's objectives were to enhance the reliability of the new Blue Gene/P operating system and to assure that it used the networks at full performance. In completing their work, the team demonstrated that a carefully designed full operating system does not incur any significant overhead for applications compared to other, more restrictive run-time systems such as MPI. For the first time, as a result of the team's work, users can share files in a completely interactive environment—encompassing the CPU and IO nodes, the login node, and the users workstation—without requiring system administrator privileges. This capability is the first of its kind for operating systems running on a supercomputer.

The next phase of the project includes investigating, measuring, and designing new operating systems and environments for next-generation HPC systems. The team is currently developing, in parallel, a unified execution model for applications and new O/S capabilities to fully exploit the flexibility given by this more flexible run-time model.

Computer Science

Performance Evaluation and Analysis Consortium End Station: Harnessing the Expertise of the Performance Community for Leadership Class Computing

PI: Patrick Worley, Oak Ridge National Laboratory
Intrepid Allocation: 8 Million Hours

The computer performance community is a critical resource for the U.S. Department of Energy's leadership class computing facilities and researchers, developing tools and performance-related infrastructure, working directly with important simulation models, and characterizing performance and providing guidance on using the facilities.

The Performance Evaluation and Analysis Consortium (PEAC) End Station, led by Patrick Worley of Oak Ridge National Laboratory, provides access to these facilities and coordinates the research activities of the performance community.

Recent contributions by PEAC researchers include porting and further development of performance diagnostic tools such as HPCToolkit, the Libra load balance analysis tool, and TAU (Tuning and Analysis Utilities) on the Blue Gene/P supercomputer at the ALCF, and the initial port of the Berkeley UPC compiler and GASNet communication layer to the Blue Gene/P. The development of a new clustering algorithm is also enabling new ways of diagnosing performance problems when using very large numbers of processors.

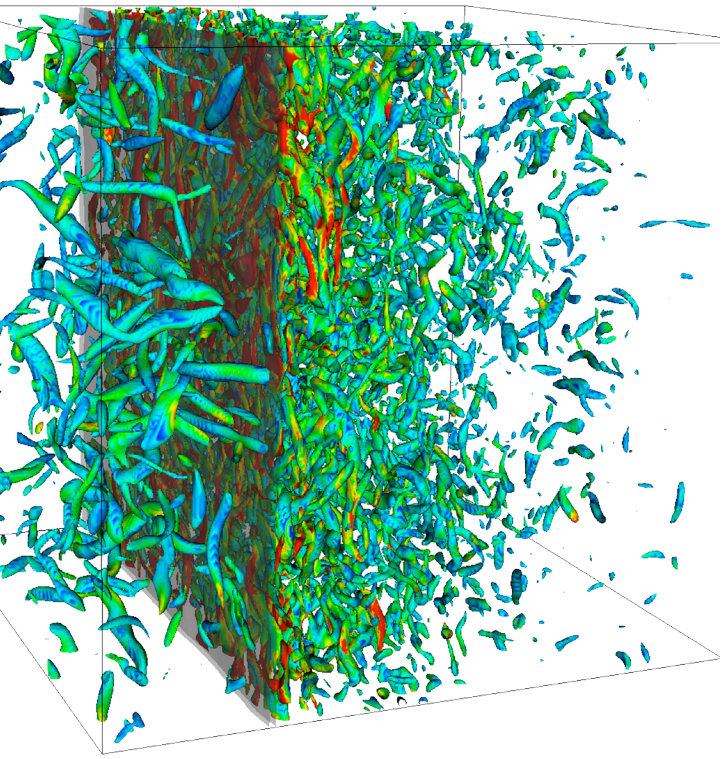
PEAC researchers used performance modeling techniques and performance data collected on the Blue Gene/P and other systems to advise the Department of Energy on its 10-year facility planning. Basic research on automated performance tuning was used to evaluate the capabilities of processor architectures used in leadership class facilities and to describe some of the software infrastructure needed to effectively exploit these capabilities. Other research focused on the performance evaluation and optimization of simulation models, including the PFLOTRAN subsurface flow model, the S3D combustion model, and FLASH astrophysics model, demonstrating the ability to use effectively over 100,000 processors of the Blue Gene/P for some models. Recent research results were reported at major computer science conferences, including ICCS, PLDI, PPoPP, and SC09 and in journal articles and book chapters.

Thanks to the work of the PEAC initiative, the Blue Gene/P operates in a more stable, efficient way and assures that research scientists can be even more effective users of this valuable resource.

Engineering

Fundamental Study of Shock/Turbulence Interaction

PI: Sanjiva Lele, Stanford University
Intrepid Allocation: 8 Million Hours



When shock waves and turbulence meet, they interact in a way that destabilizes the flow within an airplane's supersonic propulsion system. Because scientists' understanding of this phenomenon is still incomplete, they have been unable to design systems that don't sacrifice performance for stable operation. Having a better understanding will enable more accurate turbulence models and improved supersonic aircraft design.

Using the Blue Gene/P at the ALCF, a team led by Sanjiva Lele of Stanford University computed a set of canonical shock/turbulence interactions at unprecedented fidelity with sufficient resolution to accurately capture the smallest turbulent eddies. Researchers analyzed

the datasets to explain how the shock wave affects turbulence, and vice versa. They found that the post-shock turbulence rapidly becomes isotropic at the smallest scales, but the largest eddies remain anisotropic for a long distance. This result contradicts linear theory and shows that nonlinear effects are important in the post-shock evolution of the turbulence.

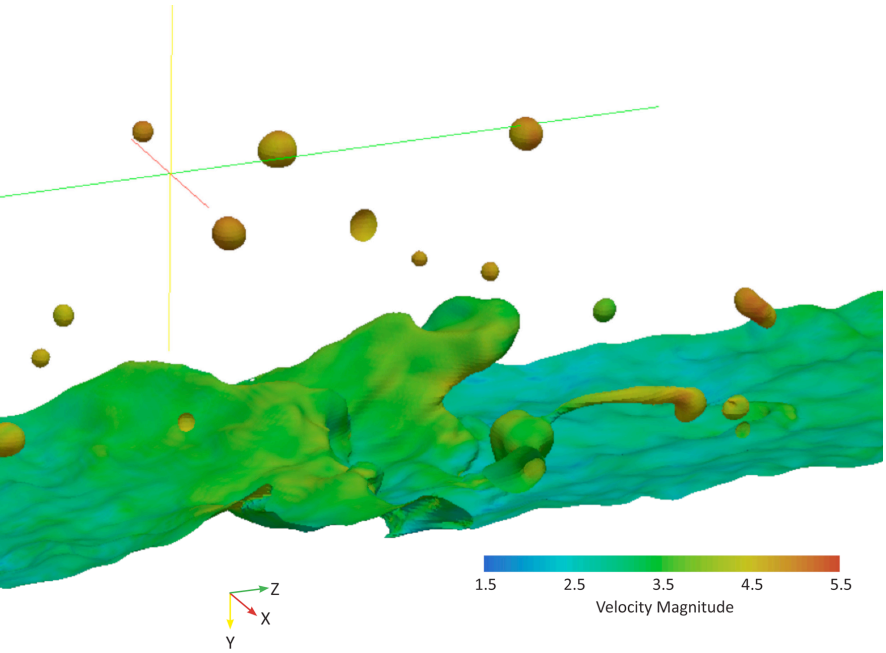
In contrast, the amplification of turbulence kinetic energy during the interaction is consistent with linear theory. The team also learned that the instantaneous shape of the shock wave is highly distorted for strong incoming turbulence, and that the turbulence can even "punch holes" in the shock wave where the compression is entirely smooth.

In the project's next phase, the team will develop robust, accurate engineering turbulence models to discover how instantaneous eddies evolve through—and behind—the shock wave.

Engineering

Petascale Adaptive CFD for Anisotropic Flows

PI: Kenneth Jansen, Rensselaer Polytechnic Institute
Intrepid Allocation: 5 Million Hours



Scientists seeking to solve complex computational fluid dynamics problems in such areas as fluid mechanics, solid mechanics, electromagnetics, and biomechanics have devised a number of partial differential equations to aid them in their research. But many questions still elude solutions because of their expense or the limitations of scalability.

Led by Kenneth Jansen of Renssalaer Polytechnic Institute, researchers used the Blue Gene/P supercomputer at the ALCF to devise a parallelization paradigm and associated protocols that enabled an implicit, unstructured mesh flow solver to achieve scalability. The techniques are amenable to other linear or nonlinear, explicit or implicit numerical methods for partial differential equations. Complex flow problems are efficiently addressed by adapting the grid to match the solution's highly anisotropic flow features.

In an abdominal aortic aneurysm model with O(108) elements, researchers achieved near-perfect strong scaling from 512 cores up to 16,384 cores of the Blue Gene/P. Similarly, on a mesh with O(10^9) elements, researchers observed near-perfect strong scaling (93% or above) for the equation-formation stage all the way to the full system scale. These findings demonstrate that it is possible to achieve strong scalability on the Blue Gene/P and suggest that even better results may be possible on the next generation of supercomputers with hundreds of thousands of cores.

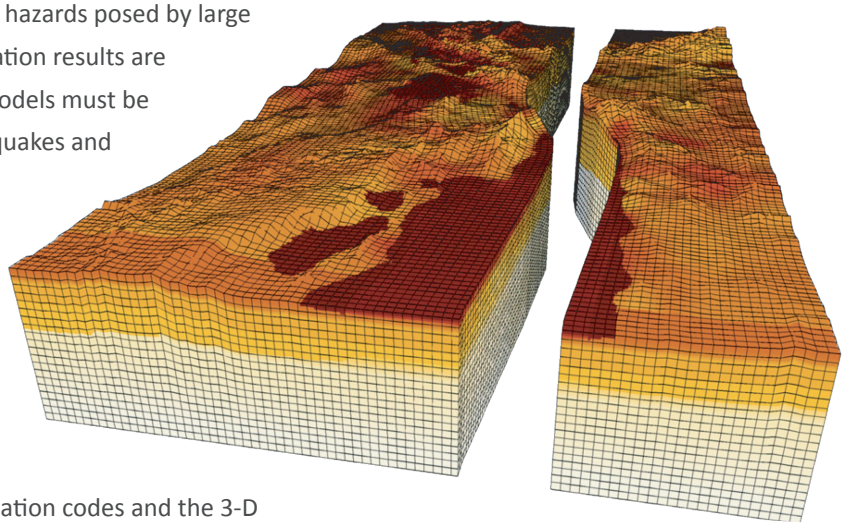
This technique has helped researchers understand complex flow physics and provides insight into such open scientific questions as active flow control on 3-D wind turbine configurations and multi-phase flows such as those occurring in accident conditions in heat exchanger tubes or core breach in Generation IV reactors.

Environmental Sciences

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

PI: Po Chen, University of Wyoming
Intrepid Allocation: 5 Million Hours

Earthquake simulations help scientists understand the hazards posed by large future earthquakes. However, before predictive simulation results are scientifically acceptable, earthquake computational models must be validated by simulating well-recorded historical earthquakes and comparing the results to observational data.



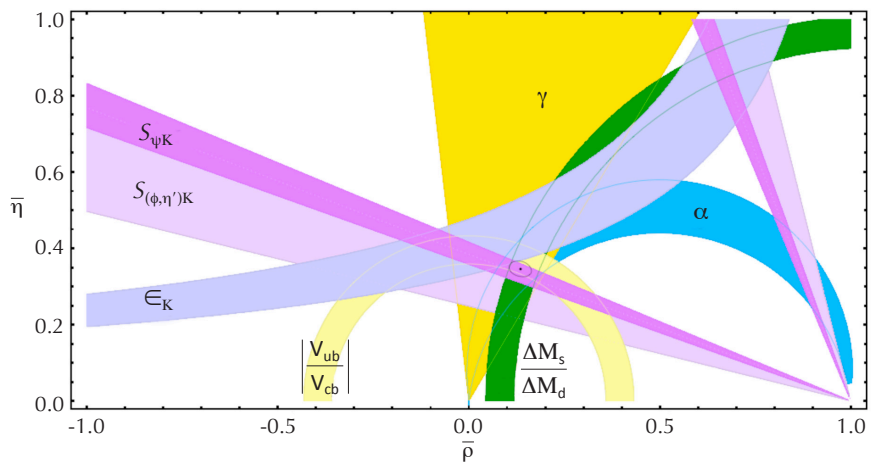
Under the direction of Po Chen of the University of Wyoming, researchers from the Southern California Earthquake Center used the Blue Gene/P supercomputer at the ALCF to simulate nearly 150 historical Southern California earthquakes. They then compared the results of their simulations against observational seismograms to confirm that their simulation codes and the 3-D structural model of California accurately replicated observed ground motions.

This large-scale validation work was performed as part of a scattering integral 3-D inversion that enabled the research team to produce an updated, improved 3-D structural model. This model will be used in future high-resolution earthquake simulations because it produces a better fit between simulation and observation. The supercomputer's speed has enabled researchers to iteratively scale up the computation model that includes simulations of historical earthquakes, validation against observation, 3-D structural model optimization, and then simulations of large future earthquakes.

Lattice Gauge Theory

Lattice QCD

PI: Paul Mackenzie, Fermi National Accelerator Laboratory
Intrepid Allocation: 67 Million Hours



Scientists have long sought to understand the basic building blocks of nature. While science understands the behavior of such particles as protons and neutrons, less is known about quarks and gluons, the even-smaller particles that make up protons and neutrons.

Because quarks and gluons interact differently than do protons and neutrons, the study of their interactions—known as quantum chromodynamics, or QCD—requires different methodology. Using the Blue Gene/P supercomputer at the Argonne Leadership Computing Facility, scientists under the direction of Paul Mackenzie at Fermilab are using a four-dimensional lattice representation of space-time to perform QCD research and build on ongoing efforts to develop a unified theory of the four fundamental forces of nature.

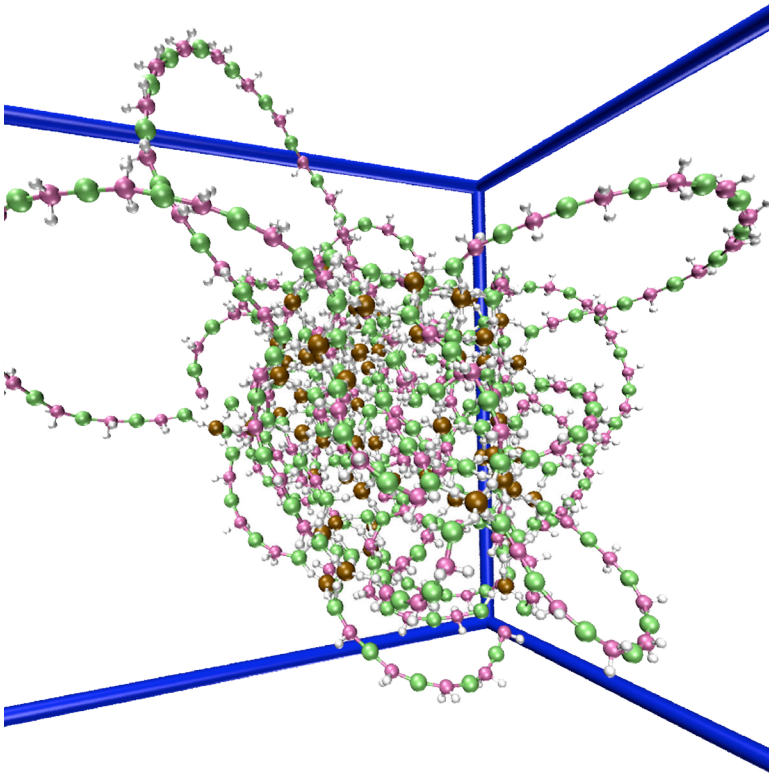
Scientists have generated gauge configurations and are using them to determine a wide range of important physical quantities in high energy and nuclear physics. With the use of the Blue Gene/P, the generation of gauge configurations has been accelerated in many cases by a factor of 5 to 10 over what was possible earlier. The team completed domain-wall configuration ensembles of lattice spacings 0.114 femtometers (fm) and 0.086 fm on the largest domain-wall lattices ever attempted: 243x64 and 32x64, respectively. In addition, researchers were also able to create the most challenging ensembles of staggered quarks to date, completing a set of runs with a lattice spacing of 0.06 and 0.045 fm.

Teams at the ALCF and elsewhere are analyzing these ensembles in studies of the decays and mixings of particles containing heavy quarks to enable major improvements in determining a number of elements of the CKM matrix. What they have learned from these configurations is providing a deeper understanding of fundamental physics.

Materials Sciences

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles

PI: Christopher Wolverton, Northwestern University
Intrepid Allocation: 1 Million Hours



Scientists continue to seek clean, renewable energy sources to reduce dependence on foreign oil. One promising energy source for cars is hydrogen. However, to make hydrogen a viable energy source, scientists must devise a two-pronged solution: They must first identify practical ways to store the hydrogen aboard the vehicle, then extract it from storage to use it. Though researchers have identified ways to safely store hydrogen within other materials, the methods are impractical for actual use.

With the Blue Gene/P supercomputer at the ALCF, a research team led by Christopher Wolverton of Northwestern University has created a "virtual laboratory" in which a predictive, physics-based modeling approach allows prospective storage materials to be tested, all on computers, before ever being synthesized in a laboratory, thus rapidly accelerating the pace of discovery.

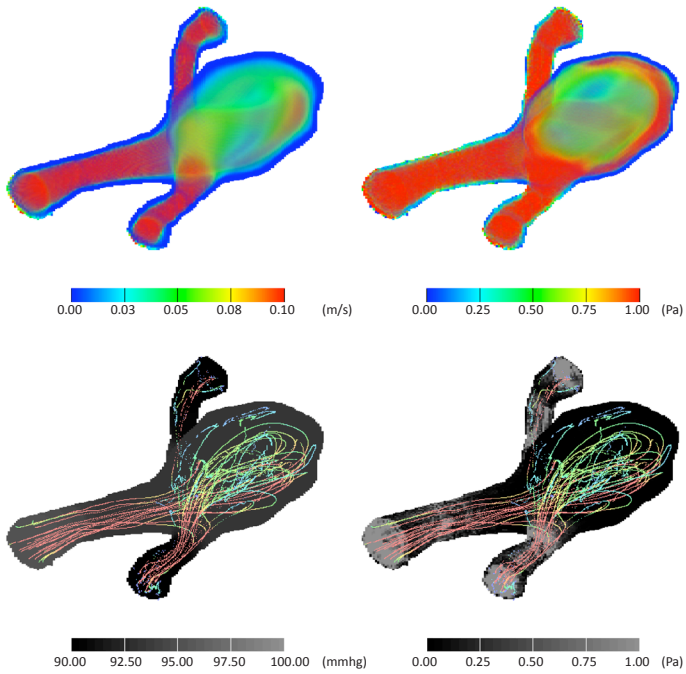
Next, researchers will use the accurate predictive power of first-principles modeling to understand the microscopic kinetic processes involved in hydrogen release and uptake. That information will aid in the design of new systems with improved properties.

This research has broad implications for many alternative energy technologies, including battery electrodes, solar electricity cells, thermoelectrics, and fuel cells. For each, computation will play a key role toward discovery.

Materials Sciences

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Understanding How Blood Flows in the Brain

PI: Peter Coveney, University College London
Intrepid Allocation: 40 Million Hours



Cardiovascular disease is the third-largest cause of death in the developed world, and it often presents as an anomaly in the brain, such as an arterio-venous malformation or aneurysm. For this reason, understanding the behavior of blood flow in the brain is a critical element in diagnosis and treatment.

Using computer simulations on the Blue Gene/P supercomputer at the ALCF, a team of scientists and clinicians led by Peter Coveney of University College London conducted virtual experiments to study cerebral blood flow at the individual patient level. Their experiments have included devising customized patient blood-flow simulations.

The researchers focused on two types of aneurysms occurring in different vessels in the brain: internal carotid artery aneurysms and pericallosal artery aneurysms. Investigators are seeking to identify relationships between the formation of these aneurysms and the patient's overall brain artery structure.

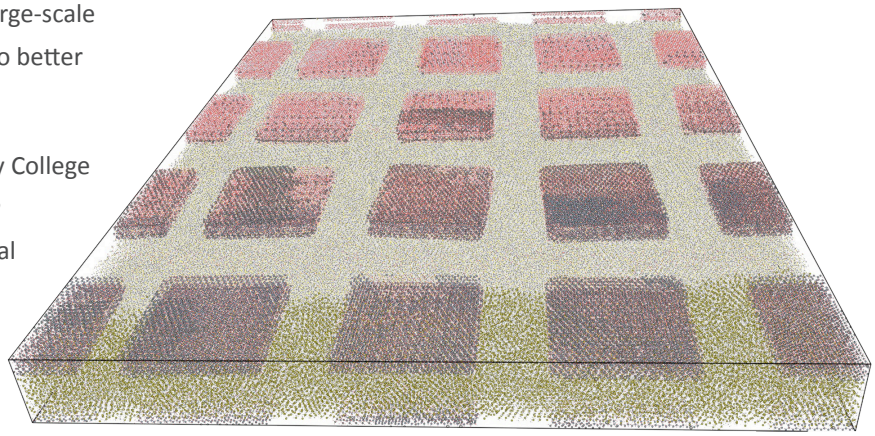
Having a computational tool that surgeons can use to examine the pressure and velocity variations in a patient's blood vessels and to predict what changes might occur as a result of interventional surgery will add immeasurably to a surgeon's "tool kit." Because patient-specific data is used as the basis of the simulation, treatments can be assessed for their effectiveness in the individual patient even before being administered, thus reducing risk and expense.

Materials Sciences

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Studying the Molecular Dynamics of Clay-Polymer Nanocomposites

PI: Peter Coveney, University College London
Intrepid Allocation: 40 Million Hours

Nanocomposites have unique attributes that make them desirable materials for many commercial uses. By creating large-scale simulations of these materials, scientists are able to better understand nanocomposites' properties.



A research team led by Peter Coveney of University College London conducted simulations on the Blue Gene/P supercomputer at the ALCF to calculate the material properties of clay platelets immersed in a polymer nanocomposite system. Tailoring the clay structure in polymers on the nanometer scale produces composites with novel material properties that have already demonstrated numerous eco-friendly applications in several industries. Once scientists fully understand the properties of nanocomposites, their use may become as widespread as that of conventional composite materials.

Through this investigation, scientists created clay-polymer nanocomposite systems comprising 10 million atoms and 16 isolated clay platelets–the first time such simulations of isolated platelets have been accomplished. A system consisting of a single platelet immersed in water allows researchers to study the process known as intercalation, in which molecules insert themselves into the spaces of another material—in this case, clay sheets.

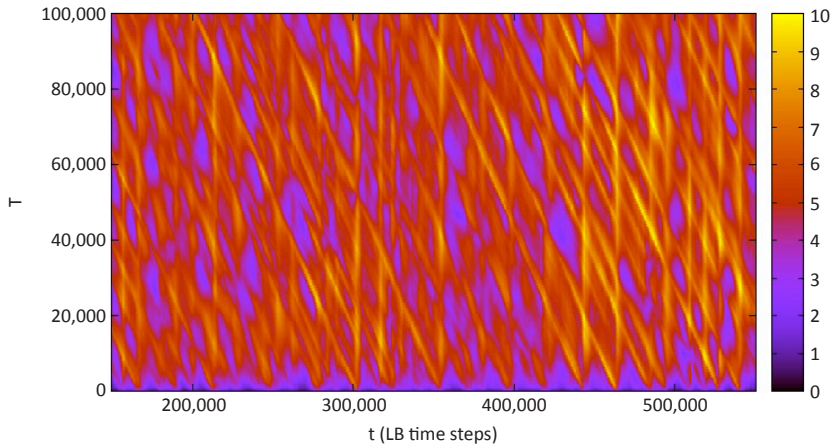
The team performed molecular dynamics simulations to a simulation time of 1ns, which will form the basis of elastic calculations to further understand the properties of clay-polymer nanocomposites. Scientists also developed a protocol for building coarse-grained simulation from all-atom simulations, from which they built a test system of 500,000 coarse-grained particles, corresponding to a 4-million-atom system.

Understanding intercalation in nanocomposites will help scientists design better processing techniques for these materials. This research will form the basis for a parallel tempering technique, which will be used to study similar, but much rarer, intercalation of large polymer molecules.

Materials Sciences

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Identifying Unstable Periodic Orbits in Navier-Stokes Equations

PI: Peter Coveney, University College London
Intrepid Allocation: 40 Million Hours



The phenomenon of turbulence is an ongoing problem and an area of continuing research. While science relies on many equations to help describe turbulence—among them the Navier-Stokes equations postulated about 150 years ago—a general method for calculating statistical averages of turbulent observations still does not exist.

Using the Blue Gene/P Intrepid supercomputer at the ALCF to carry out simulations, scientists led by Peter Coveney of University College London are locating and characterizing Unstable Periodic Orbits (UPOs) described by the Navier-Stokes equations. Their goal is to revolutionize the statistical prediction of turbulent fluid flows using a novel four-dimensional approach that is parallel in both space and time.

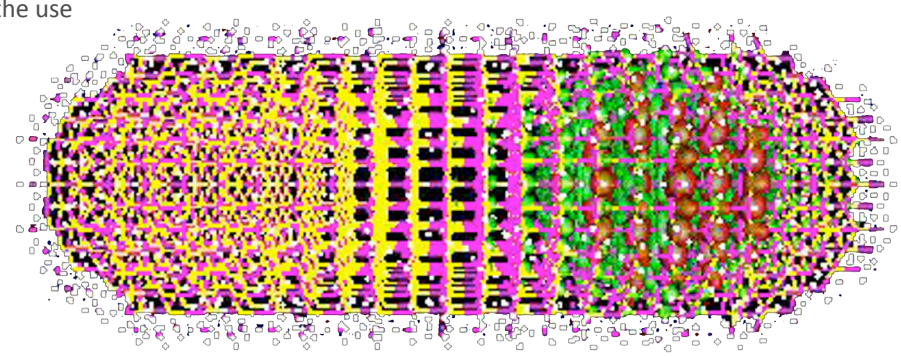
Previously, scientists identified Navier-Stokes UPOs by using a "shooting" algorithm, whereby the fluid equations are integrated forward in time as the inner loop of a Newton-Raphson solver whose aim is to match the initial and final conditions. With their more efficient variational approach, the research team has used Intrepid to validate its numerical procedures and has been able to extend those results and catalog UPOs for chaotic and turbulent systems. Researchers investigated different relaxation schemes, such as gradient descent and conjugate gradients, and optimized parameters to facilitate convergence.

This work is believed to represent the world's first trials of a space-time minimization procedure designed to locate UPOs on a high-dimensional dynamical system.

Materials Sciences

Linear Scale Electronic Structure Calculations for Nanostructures

PI: Lin-Wang Wang, Lawrence Berkeley National Laboratory
Intrepid Allocation: 1 Million Hours



Because of their high cost and poor efficiency, the use of solar cells has not yet become widespread. Scientists believe nanomaterials—that is, materials whose unique properties can be leveraged at the molecular level—represent the best chance for optimizing solar cell technology. First, however, scientists must gain an understanding of the internal electric field in these nanostructures, caused either by bulk and surface dipole moments or by piezoelectric effects.

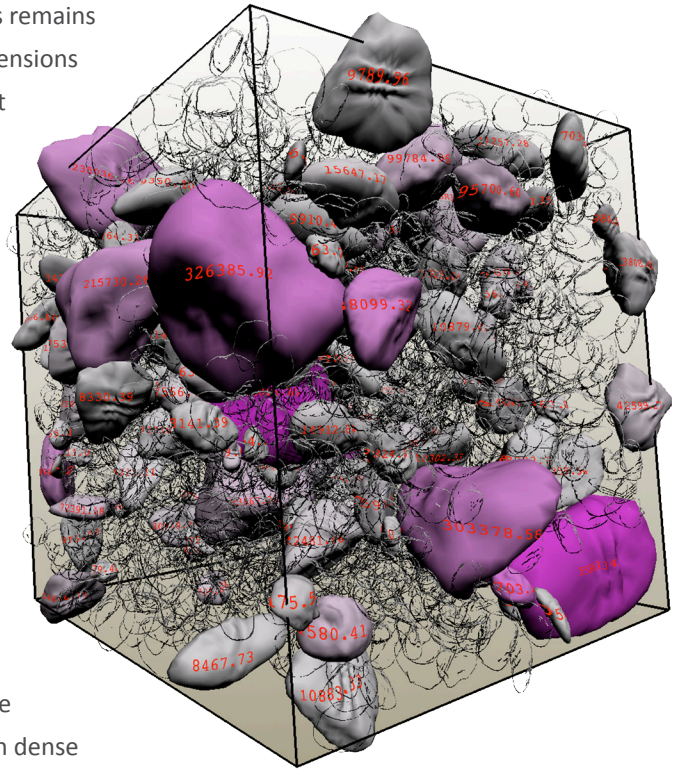
A research team led by Lin-Wang Wang of Lawrence Berkeley National Laboratory is using the Blue Gene/P supercomputer at the ALCF to carry out large-scale computations to calculate the charge density and electric field inside a 5,000-atom nanostructure. Their work has revealed the discovery of surprisingly large electric fields in nanorods, often caused by dipole moments from the side surfaces. Such electric fields will completely separate the electron and hole to opposing sides of the nanorod.

Scientists also have determined that the piezoelectric effect is relatively small. In the project's next phase, researchers will search for charge compensation mechanisms that would counterbalance the internal electric fields in these nanorods.

Materials Sciences

Modeling the Rheological Properties of Concrete

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



The flow behavior, or rheology, of dense suspensions remains something of a mystery to researchers because suspensions are complex and are not easily understood. Yet, what scientists learn from studying suspensions may have technological application across a wide and varied range of industries, from coatings and construction to foods and pharmaceuticals.

A team led by William L. George at the National Institute of Standards and Technology is using the Blue Gene/P supercomputer at the ALCF to study the flow of dense suspensions like concrete. The team has created computational models that account for the dense packing of particles with broad variations in shape and size along with interparticle interactions.

Preliminary findings suggest that particle contacts are an important factor in controlling the onset of flow in dense suspensions. Also, for some suspensions, the shear rates between aggregates strongly determine their rheological properties. The team successfully validated its results against physical experiments.

The project's next phase will include a study of the effect of varying particle shape by mixing different classes of particles that are representative of realistic materials and comparing the effect of Newtonian vs. non-Newtonian fluid matrices on the rheological behavior of suspensions.

Nuclear Energy

Predictions of Thermal Striping in Sodium-Cooled Reactors

PI: Andrew Siegel, Argonne National Laboratory
Intrepid Allocation: 7.5 Million Hours

Computer simulation is helping to optimize the design of a new generation of Advanced Recycling Reactors, or ARRs. These reactors help address global concerns regarding nuclear waste management and 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 the ability to predict thermal striping—that is, the phenomenon that occurs when partially mixed streams of sodium coolant expose structural materials to cyclic thermal stresses, causing fatigue and limiting their lifetime.

Traditionally, designers have relied on data from instrumented experiments, but such data is expensive, difficult to collect, and greatly limited in its spatial fidelity and adaptability to scope design space. Argonne National Laboratory researchers, under the direction of Andrew Siegel, are using the Blue Gene/P supercomputer at the ALCF to carry out the first detailed numerical experiments of thermal striping on realistic reactor geometries. Their advanced simulations enable detailed analysis of the flow distribution and heat transfer characteristics of "fast neutron reactors."

These reactors hold great promise for the energy future of the United States, reducing nuclear waste and significantly extending nuclear fuel resources. The team's thermal striping calculations are expected to be validated by another project also under way at Argonne at this time.

The team's work is expected to help further scientists' understanding of a broad range of poorly understood reactor phenomena.

Nuclear Physics

Computational Nuclear Structure

PI: David Dean, Oak Ridge National Laboratory
Intrepid Allocation: 10 Million Hours

Although scientific research has greatly enhanced our understanding of nuclear structure, much more remains to be learned. A team of researchers, led by David Dean of Oak Ridge National Laboratory, is pursuing this study. The team represents a collaboration of scientists from Argonne National Laboratory, Iowa State University, and the University of Tennessee. The team is using the supercomputing capabilities of the Blue Gene/P at the ALCF and the Cray XT4 at Oak Ridge National Laboratory.

Researchers used several complementary techniques—including Green's Function Monte Carlo, Hamiltonian Diagonalization (the No Core Shell Model), and Coupled-Cluster methods—to perform calculations of both structural and reaction properties of light and medium mass nuclei and the three-nucleon force.

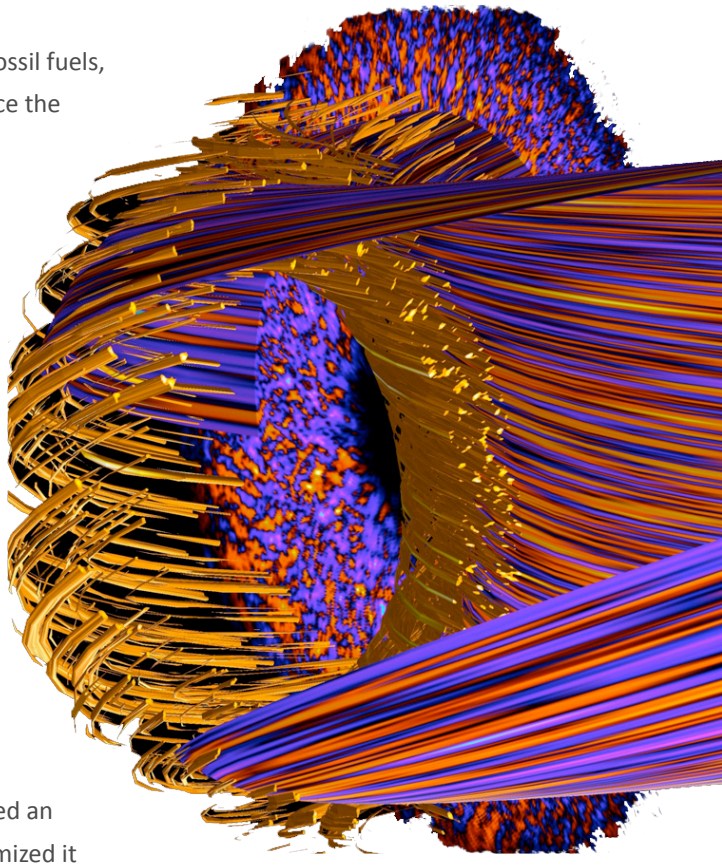
This project explores, for the first time, the role of the three-nucleon force in substantially heavier nuclei such as 16O, 40Ca, and 56Ni.

The team is also using the supercomputers to replicate the phenomenon known as triple-alpha burning, or ”helium burning.” Their work is expected to shed light on this vital process—essential to life on earth—in which stars fuse helium, carbon, and oxygen nuclei after exhausting their hydrogen fuel.

Plasma Physics

High-Resolution Global Simulation of Plasma Microturbulence

PI: William Tang, Princeton Plasma Physics Laboratory
Intrepid Allocation: 6 Million Hours



As the world seeks cleaner energy alternatives to fossil fuels, nuclear fusion becomes increasingly attractive. Since the early 1950s, researchers have studied fusion—the power source of the sun and other stars. Although progress has been impressive, remaining issues hindering our ability to deliver commercial fusion power include the key problem of microturbulence—the primary means by which heat leaks out of the magnetic “trap” designed to confine hot plasma gas. Understanding and controlling microturbulence is key to achieving the efficiency needed to ensure the practicality of fusion power plants.

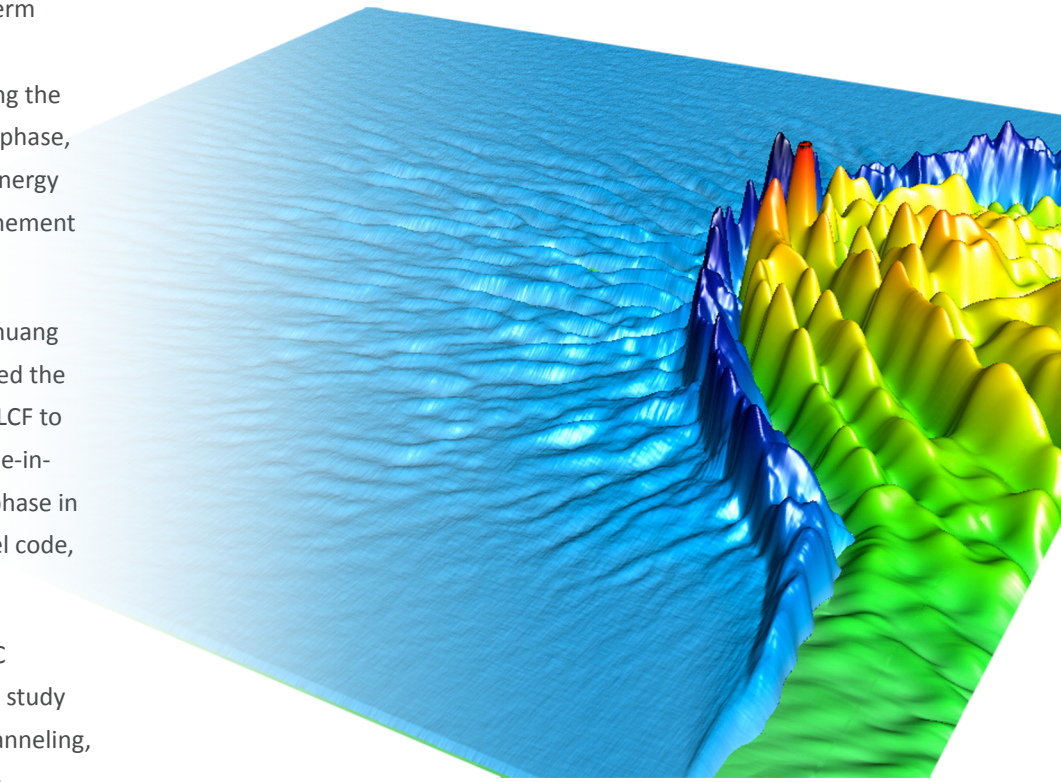
Using predictive computational models has enabled unparalleled gains in understanding microturbulence. Led by scientists from the Princeton Plasma Physics Laboratory (William Tang and Stephane Ethier) a research team has developed an advanced 3-D global, particle-in-cell code and optimized it using the Blue Gene/P at the ALCF to examine the effect of collisions on the plasma confinement properties. The supercomputer’s multi-core processors enable unprecedented higher-resolution global simulations of plasma microturbulence in a multi-dimensional phase-space.

The long-time simulations carried out on the Blue Gene/P not only provide evidence that collisional dynamics cannot be ignored but that a larger number of particles per cell is necessary to achieve phase-space resolution. Such insights help scientists understand and mitigate the influence of microturbulence on efficient magnetic confinement of fusion-grade plasmas. In the project’s next phase, the team will examine the key question of how trends observed in current simulations might be affected as plasma size increases.

Plasma Physics

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

PI: Chuang Ren, University of Rochester
Intrepid Allocation: 1.5 Million Hours



Fusion energy is regarded as a long-term energy solution that is both safe and environmentally friendly. By separating the compression phase from the ignition phase, fast ignition aims to increase fusion energy gain and the viability of inertial confinement fusion as an energy source.

Researchers under the direction of Chuang Ren of the University of Rochester used the Blue Gene/P supercomputer at the ALCF to carry out first-principles-based Particle-in-Cell (PIC) simulations of the ignition phase in fast ignition, using a massively parallel code, OISRIS.

Using two- and three-dimensional PIC simulations, researchers were able to study the ignition phase, including laser channeling, hot electron generation, and electron transport, with unprecedented scale and detail. They found that ultra-intense lasers can be used to create a clean channel to improve the transmission of the ignition pulse and to generate electrons within the energy range suitable to ignite the target. Together, these results open up a new regime of fast ignition using ultra-intense lasers—something once regarded as unfeasible.

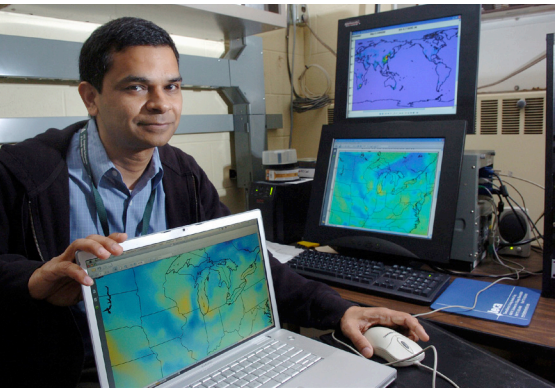
By leveraging increased computer resources and improved code capability, researchers will perform even more realistic simulations. A key issue is magnetic collimation in the dense plasma region, where collisions are important. In addition, they will study laser-induced relativistic shocks important to fast ignition and to astrophysics.

DIRECTOR'S DISCRETIONARY

Climate Research

Large-Scale Parameter Sweeps Procedures for Developing Condensed Aerosol Schemes for Climate Models

PIs: V. Rao Kotamarthi, Argonne National Laboratory and T. Stef-Praun, Computation Institute, University of Chicago
Director's Discretionary Allocation: 60,000 Hours



Aerosol physical and chemical process models involve multiple physical parameters, chemical pathways, multiple components, and microphysical processes. Representation of aerosols in climate models has proved to be particularly challenging as a result. The increased computational burden from including aerosol processes models in all their details has not yet been justified. A need exists for developing approximate approaches to develop and represent condensed forms of aerosol formation, portioning between various chemical compositions, and the effect of atmospheric parameters on these processes. In addition, there is a need to develop a condensed chemical mechanism for represent secondary organic aerosols from all the currently hypothesized organic gas precursor chemical pathways.

Researchers have implemented a large-scale parameter sweep procedure at the Argonne Leadership Computing Facility using a 1-D atmospheric chemistry and aerosol chemistry-physics model on the IBM Blue Gene/P supercomputer. The chemistry schemes implemented include RACM, CB4, and SAPRC-99 for volatile organic compounds; JPL for inorganic chemistry; SORGAM for secondary organic aerosols; FAST J for photolysis rates; and ISOROPIA for thermodynamic equilibrium calculations for inorganic aerosols. In addition, this 1-D model includes a PBL dynamics model based on k epsilon theory, achieving a 2.5 level closure for the Reynolds stress in calculating turbulence in the PBL. The PBL is very finely resolved in this 1-D model, which has been used to investigate fast reactions and interactions with PBL turbulence. The coupling of this model with the climate model radiation code CRM allows researchers to investigate radiative feedbacks from selected aerosols for direct calculation of radiative forcing.

DIRECTOR'S DISCRETIONARY

The equations near the top of Figure 1 show the equilibrium relationship between these three gas phase constituents and the parameters that influence this equilibrium. The second half of the figure shows the possible combinations of parameters that need to be studied for fully analyzing this system. There is a minimum of 10 parameters in this system and one can imagine creating a table for each parameter taking a minimum of 100 values. This would create a matrix of 10 x 100, and to perform full analysis of this system for each value of the parameter, researchers have to do a number of combinations. The full calculations are of the order 3 million needed for a 10 x 10 system with no repetition allowed. This is a large number of calculations that could take years to perform. Once fully implemented on the new Blue Gene/P, this calculation can be completed in less than a day. Preliminary analysis of the results from these simulations has been performed.

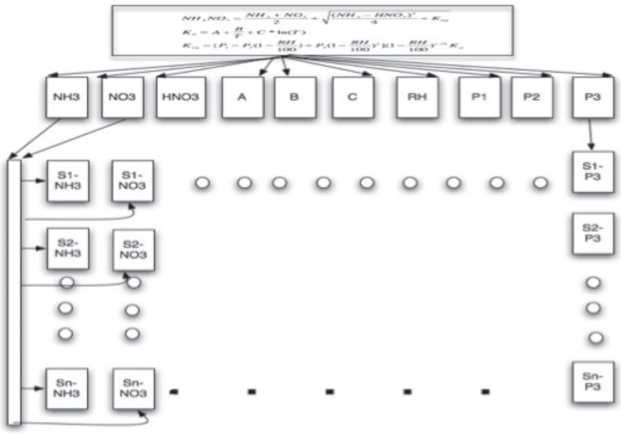


Figure 1

A 500-member simulation was performed using the latin hypercube sample. Each model simulation was initialized using the concentrations of ammonia, NO_x, temperature and relative humidity (RH). The analysis indicated that the amount of nitrate formation can vary between 10% and 15% based on changes in these four variables alone in the model after about two hours of simulation time. Each model was simulated for 36 hours from the initial time, which was set to approximately 4 hours local time at locations corresponding to the Midwestern United States on a summer day. (See Figure 2.)

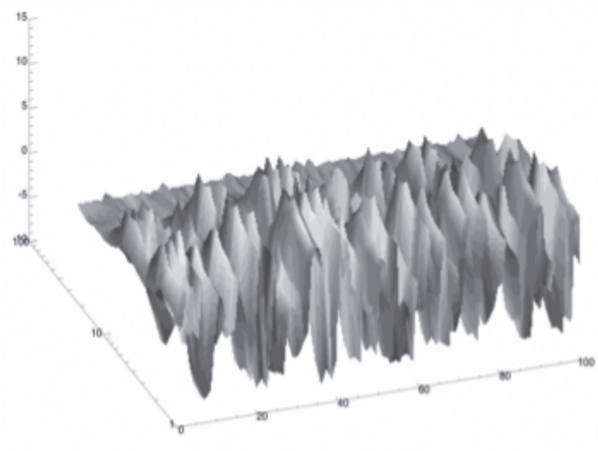


Figure 2

Further simulations to test the entire range of parameter space described in Figure 1 will be performed and analyzed over the next few months.

The parameter sweep procedure uses a workflow management tool known as SWIFT in combination with a latin hypercube sampling procedure implemented for a multi-parameter aerosol system describing the NH3-NO3-SO4 inorganic system. Results from these parameter sweeps, ranging over 1,000 to 100,000 simulations and covering a wide range of physical, chemical, and input parameters to this aerosol processes in the 1-D model.

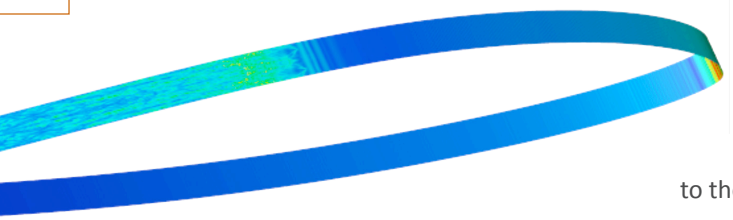
DIRECTOR'S DISCRETIONARY

Computational Fluid Dynamics/Aero-Acoustics

Using Large-Eddy Simulations to Create Quiet Wind Turbines

PI: Anurag Gupta, GE Global Research
Director's Discretionary Allocation: 13.1 Million Hours

Reducing aerodynamic noise is critical for the continued viability of next-generation "green" low-carbon/greenhouse gas emission energy systems such as wind turbines. Scientists at GE Global Research are investigating ways to reduce airfoil trailing edge noise, a key component in wind turbine noise, by developing computational methods to characterize it from first principles.



Using Large Eddy Simulation (LES) methods on the ALCF's Blue Gene/P, the team has demonstrated the ability to successfully predict such key flow phenomena as natural laminar flow transition at realistic flight-scale Reynolds numbers. Refinements to the higher-order flow solver and improved code scalability were needed to accurately predict boundary layer characteristics that are a first step in characterizing the noise generation and propagation mechanism for trailing edge noise. Such hard-to-measure details and sources of noise are key to developing models that can be used in design tools. With massively parallel, high performance computing enabling such simulations, GE's ability to design larger, but quieter wind turbine blades is accelerated.

With noise being one of the principal barriers in growing rotor diameters, and hence increasing renewable energy yields from the world's wind resources, this capability will provide a significant tool in tackling earth's greenhouse gas problems.

High-Energy Physics

Computation of Electron Cloud Diagnostics and Mitigation in the Main Injector

PIs: Paul LeBrun, Fermi National Accelerator Laboratory and Seth Veitzer, Tech-X Corporation
Director's Discretionary Allocation: 0.6 Million Hours

Future experiments to study high energy physics require the construction of new, high-intensity particle accelerators that are pushing the frontiers of accelerator design. Electron cloud effects are considered to be one of the most important factors that will limit machine performance for high-intensity accelerators, and electron cloud mitigation methods can have a large influence on the cost and design of such accelerators. Researchers have recently developed a new diagnostic technique that uses microwaves to measure electron cloud densities. At Fermilab, the performance-degrading aspects of electron clouds are a major concern for the Lab's planned upgrade of its Main Injector to 2 MW of beam power.

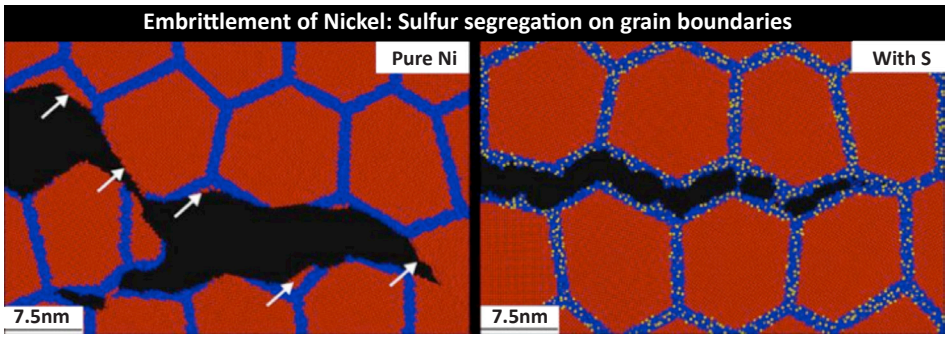
DIRECTOR'S DISCRETIONARY

The VORPAL software from the Tech-X Corporation and the high-performance capabilities of the Blue Gene/P at the Argonne's Leadership Computing Facility have been used to determine phase shifts induced in injected microwave fields, as a function of electron cloud density in the Main Injector. Inversion of the relationship between electron cloud parameters and induced phase shifts allows researchers to predict electron cloud density and evolution over many bunch periods. Long time-scale simulations using Blue Gene have allowed them to measure cloud evolution patterns under the influence of beam propagation with realistic physical parameterizations, such as elliptical beam pipe geometry, self-consistent electromagnetic fields, space charge, secondary electron emission, and the application of arbitrary external magnetic fields. Simultaneously, the researchers are able to simulate the effectiveness of various mitigation techniques, such as surface coating and the application of confining magnetic fields. These simulations provide quantitative information for electron cloud diagnostic, instrumentation, and future accelerator designs.

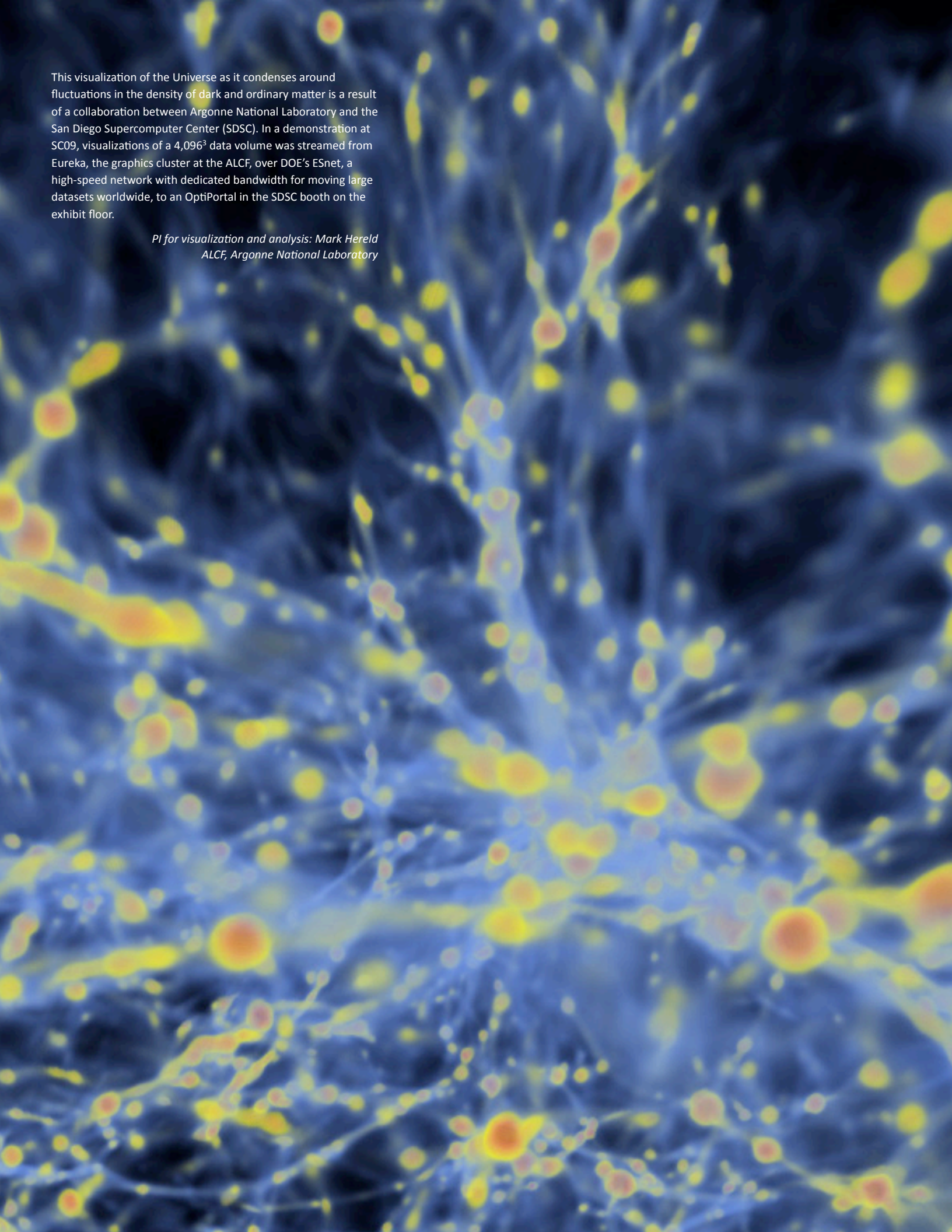
Materials Sciences

Modeling Nickel Fractures and Next-Generation Reactors

PI: Priya Vashishta, University of Southern California
Director's Discretionary Allocation: 30 million hours



A multidisciplinary team of physicists, chemists, materials scientists, and computer scientists made innovations in simulation methods and parallel computing technologies to perform the largest-ever (48 million atoms), chemically reactive molecular dynamics simulation on 65,536 IBM Blue Gene/P processors at the Argonne Leadership Computing Facility. The team answered a fundamental question encompassing chemistry, mechanics, and materials science: How a minute amount of impurities segregated to grain boundaries of a material essentially alters its fracture behavior. The researchers simulated the introduction of small amounts of sulfur into the boundaries between nickel grains to investigate a material property known as "embrittlement." Seeing how different configurations of nickel function at these exceptionally small scales helps them understand the basic chemistry that will expedite the development of next-generation nuclear reactors.



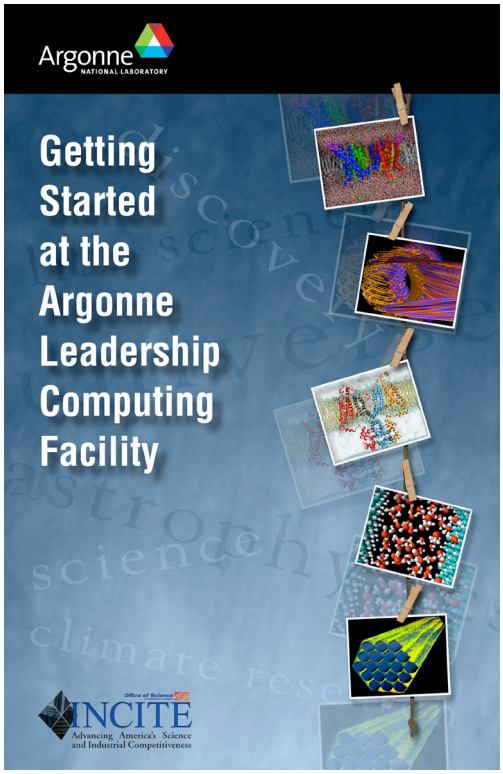
This visualization of the Universe as it condenses around fluctuations in the density of dark and ordinary matter is a result of a collaboration between Argonne National Laboratory and the San Diego Supercomputer Center (SDSC). In a demonstration at SC09, visualizations of a $4{,}096^3$ data volume was streamed from Eureka, the graphics cluster at the ALCF, over DOE's ESnet, a high-speed network with dedicated bandwidth for moving large datasets worldwide, to an OptiPortal in the SDSC booth on the exhibit floor.

PI for visualization and analysis: Mark Hereld
ALCF, Argonne National Laboratory

OUTREACH AND EDUCATION

In 2009, the Argonne Leadership Computing Facility hosted a series of workshops, a webinar, and an open house to educate users and participated in key computing conferences.

ALCF "Getting Started" Workshop Benefited INCITE Researchers



Researchers representing eight INCITE projects benefited from a February 10–11 INCITE "Getting Started" Workshop held by the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory. Scheduled each year to occur shortly after the DOE INCITE awards are announced, the workshop is specifically designed to give new projects a "jump start" by providing users with assisted hands-on training in porting and tuning their applications on the Blue Gene/P supercomputer, plus a complete overview of ALCF services and resources available to them. In addition, the workshop featured a special session on the Eureka system, which provides visualization and data analytics to transform data from the Blue Gene/P into useful knowledge. Eureka offers more than 111 teraflops of computer power and more than 3.2 terabytes of RAM (5% of Intrepid RAM).

"Introduction to BG/P" Workshop Targeted at Non-INCITE Projects

The Argonne Leadership Computing Facility (ALCF) held an "Introduction to BG/P" Workshop for non-INCITE project users on March 10-11 at Argonne National Laboratory. The workshop provided these users with an overview of ALCF services and resources, technical details on the ALCF Blue Gene/P architecture, and hands-on assistance in porting and tuning users' applications onto the Blue Gene/P. It offered an excellent opportunity to interact with the ALCF staff and learn more about the Blue Gene/P machine, as well as data analytics and visualization capabilities at the ALCF. Attendees took a tour of the Interim Supercomputing Support Facility and particularly appreciated the hands-on experience offered at the workshop.

Ready, Set, "Leap to Petascale" Workshop

At the Argonne Leadership Computing Facility "Leap to Petascale" workshop on May 27–29, users learned about the petascale resources available to them. ALCF performance engineers helped users scale and tune their applications on the Blue Gene/P's 40 racks.

INCITE Proposal Writing Webinar Provided Tips for Quality Proposals

DOE's INCITE program—jointly managed by the Argonne and Oak Ridge Leadership Computing Facilities—made available more than one billion processing hours for 2010. A June 2nd Proposal Writing webinar sponsored by the program helped candidates craft the most effective INCITE proposals to garner their share of these hours. Katherine Riley, team lead of the Argonne Leadership Computing Facility's (ALCF's) Catalyst group, and Bronson Messer, computational astrophysicist in the Scientific Computing Group at Oak Ridge's National Center for Computational Sciences, provided suggestions to improve the quality of the proposal submissions.

World-Class Computing Capability Highlighted at CSGF Conference

DOE Computational Science Graduate fellows are part of an innovative group learning to solve problems outside traditional boundaries. An annual conference makes it possible for these leaders to get together, share ideas, support one another, and discover the research opportunities at DOE laboratories.

At the 2009 Computational Science Graduate Fellowship (CSGF) Conference held July 14-16 in Washington, DC, Argonne's computational science research efforts were highlighted in a wide range of scientific disciplines at the Department of Energy Laboratory Poster Session and Fellows Poster Session. Argonne experts from the Computing, Environment, and Life Sciences directorate; Argonne Leadership Computing Facility; and Mathematics and Computer Science Division participated in the poster sessions.

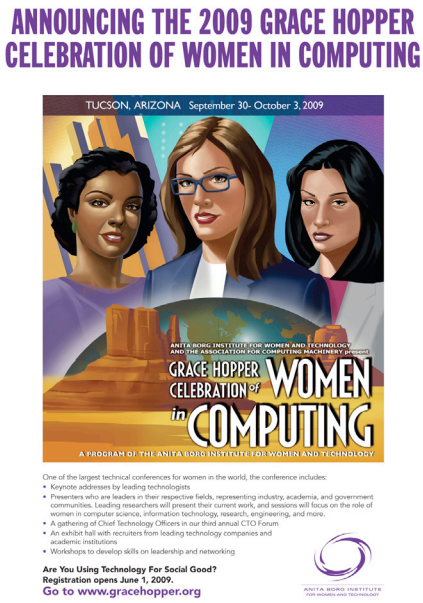
Blue Gene/P's Capabilities Showcased at Argonne Open House

The Argonne Leadership Computing Facility (ALCF) showcased the Blue Gene/P's speed, storage, and performance capabilities at the Argonne National Laboratory Open House on August 29. Overall, nearly 100 engaging exhibits, demonstrations, tours, and presentation informed the public of Argonne's research at the Open House.

"Performance Evaluation Using TAU" Workshop Aided BG/P Users

On September 22-23, the Argonne Leadership Computing Facility (ALCF) sponsored "Performance Evaluation Using TAU," a two-day, hands-on workshop for Blue Gene/P users. Led by Sameer Shende, ParaTools, Inc., and aided by hands-on help from ALCF staff members, computational scientists evaluated the performance of their parallel, scientific applications on the Blue Gene/P with the TAU Performance System®. The scientists learned how to use TAU to collect and analyze performance data to enhance the scalability of their applications. The workshop was very well received by the participants. In fact, one attendee plans to add the TAU manual distributed at the workshop to performance tools documents.

Grace Hopper Conference Recognized Women's Key Role in Defining Technology

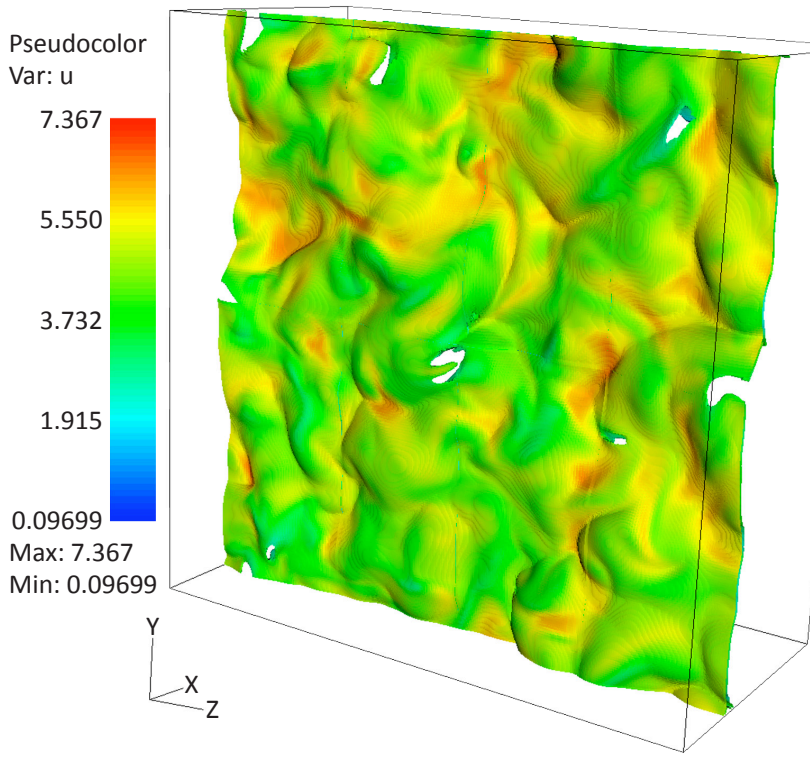


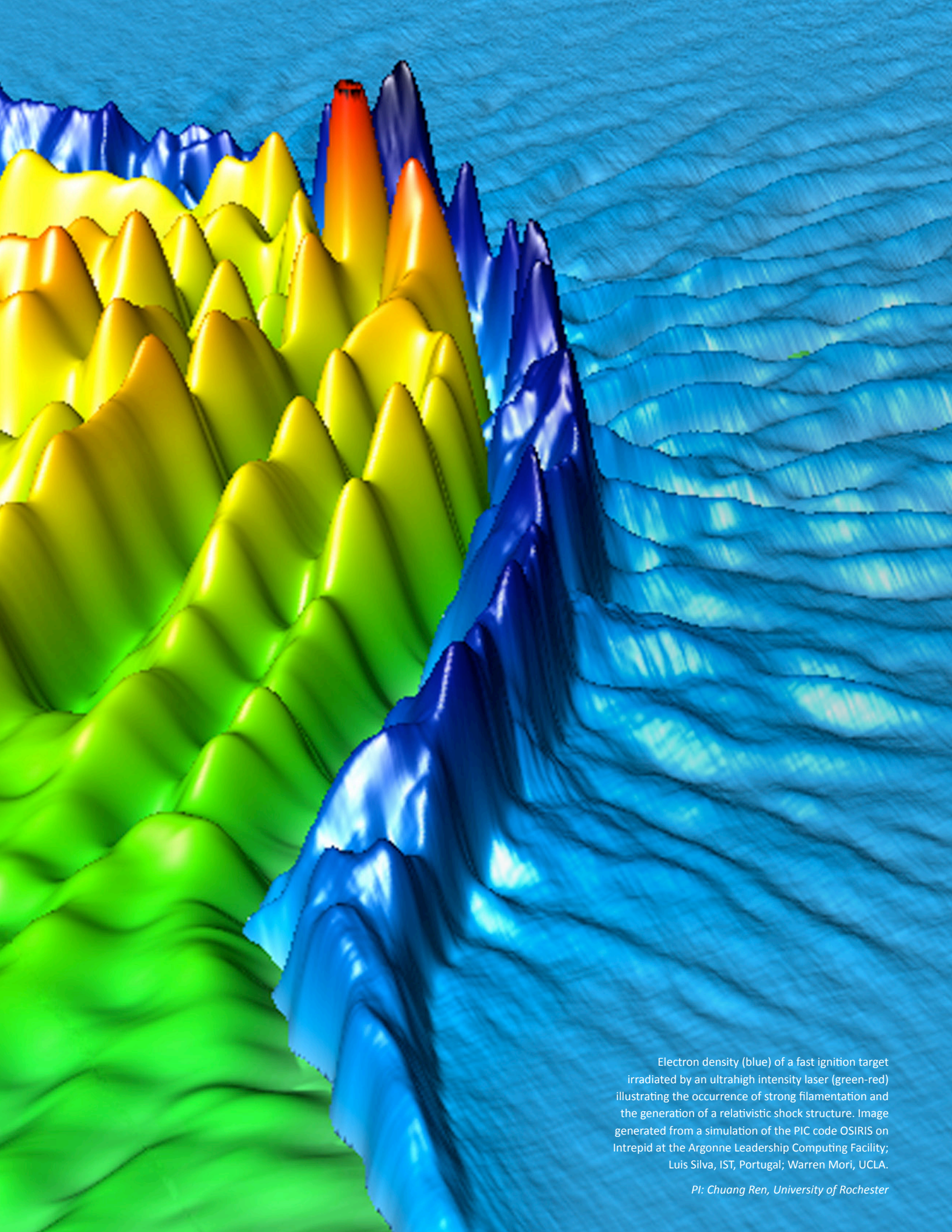
The 9th Annual Grace Hopper Celebration of Women in Computing Conference, held September 30-October 3 in Tucson, Arizona, focused on "Creating Technology for Social Good." The world's largest gathering of women in computing recognized the significant role that women play in defining technology used to solve social issues. Conference presenters were leaders in their respective fields, representing industry, academia, and government. In 2009 Argonne's Computing, Environment, and Life Sciences directorate, along with the Leadership Computing Facility, Computing and Information Systems, Mathematics and Computer Science, and Human Resources divisions, were Bronze sponsors of the conference.

Argonne Staff Engaged in Multiple SC09 Activities

Argonne National Laboratory staff presented a wide variety of papers, workshops, Birds-of-a-Feather (BOF) sessions, tutorials, and posters at SC09 on November 14-20 in Portland, Ore. Papers covered such topics as Terascale Data Organization for Discovering Multivariate Climatic Trends, a Configurable Algorithm for Parallel Image-Compositing Applications, and I/O Performance Challenges at Leadership Scale. Workshops focused on Many-Task Computing on Grids and Supercomputers (MTAGS), Grid Computing Environments (GCE) 2009, and Using Clouds for Parallel Computations in Systems Biology. BOF sessions promoted stimulating discussions on Python for High Performance and Scientific Computing; MPICH: A High-Performance, Open-Source MPI Implementation; HPC Saving the Planet, One Ton of CO_2 at a Time; International Exascale Software Program; and CIFTS: A Coordinated Infrastructure for Fault-Tolerant Systems.

Tutorials educated attendees on Python for High Performance and Scientific Computing, Parallel I/O in Practice, Configuring and Deploying GridFTP for Managing Data Movement in Grid/HPC Environments, Designing High-End Computing Systems with InfiniBand and 10-Gigabit Ethernet, InfiniBand and 10-Gigabit Ethernet for Dummies, Application Supercomputing and the Many-Core Paradigm Shift, and Advanced MPI. In addition to printed posters presented, a comprehensive array of electronic posters and research highlights were displayed at the Argonne exhibit.





Electron density (blue) of a fast ignition target irradiated by an ultrahigh intensity laser (green-red) illustrating the occurrence of strong filamentation and the generation of a relativistic shock structure. Image generated from a simulation of the PIC code OSIRIS on Intrepid at the Argonne Leadership Computing Facility; Luis Silva, IST, Portugal; Warren Mori, UCLA.

PI: Chuang Ren, University of Rochester

2010 INCITE RESEARCH PROJECTS

In 2010, 35 projects in a wide range of scientific disciplines were awarded approximately 646 million supercomputer processor-hours on Intrepid at the ALCF through DOE's ASCR Innovative and Novel Computational Impact on Theory and Experiment Program (INCITE). Of these, 16 projects were renewed from 2009, and 19 are new projects. Projects receiving INCITE awards utilize complex simulations to accelerate discoveries in ground-breaking technologies.

Biological Sciences

Computational Protein Structure Prediction and Protein Design
David Baker, University of Washington
Intrepid Allocation: 50 Million Hours

Protein-Ligand Interaction Simulations and Analysis
T. Andrew Binkowski, Argonne National Laboratory
Intrepid Allocation: 25 Million Hours

Millisecond Molecular Dynamics of Chaperoning of Unfolded Polypeptide Chains by HSP70
Harold Scheraga, Cornell University
Intrepid Allocation: 6 Million Hours

Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions
Igor Tsigelny, University of California—San Diego
Intrepid Allocation: 5 Million Hours

Chemistry

High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels
Jacqueline Chen, Sandia National Laboratories
Intrepid Allocation: 2 Million Hours

Molecular Simulation of Complex Chemical Systems
Christopher Mundy, Pacific Northwest National Laboratory
Intrepid Allocation: 2 Million Hours

Large Eddy Simulation of Two-Phase Flow Combustion in Gas Turbines
Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Intrepid Allocation: 8 Million Hours

Prediction of Bulk Properties Using High-Accuracy *Ab Initio* Methods Interfaced with Dynamical Calculations
Theresa Windus, Ames Laboratory
Intrepid Allocation: 8 Million Hours

Computer Science

Scalable System Software for Performance and Productivity
Ewing Lusk, Argonne National Laboratory
Intrepid Allocation: 5 Million Hours

BG/P Plan 9 Measurements on Large-Scale Systems
Ronald Minnich, Sandia National Laboratories
Intrepid Allocation: 1 Million Hours

Performance Evaluation and Analysis Consortium End Station
Patrick H. Worley, Oak Ridge National Laboratory
Intrepid Allocation: 8 Million Hours

Earth Science

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz
Thomas Jordan, Southern California Earthquake Center
Intrepid Allocation: 7 Million Hours

Climate-Science Computational End Station Development and Grand Challenge Team
Warren Washington, National Center for Atmospheric Research
Intrepid Allocation: 30 Million Hours

Energy Technologies

Advanced Reactor Thermal Hydraulic Modeling
Paul Fischer, Argonne National Laboratory
Intrepid Allocation: 30 Million Hours

Petascale Particle-In-Cell Simulations of Fast Ignition
John Tonge, University of California—Los Angeles
Intrepid Allocation: 7 Million Hours

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air
Jack Wells, Oak Ridge National Laboratory
Intrepid Allocation: 12 Million Hours

Engineering

Petascale Adaptive Computational Fluid Dynamics for Applications with High Anisotropy
Kenneth Jansen, Rensselaer Polytechnic Institute
Intrepid Allocation: 10 Million Hours

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

Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability
Sanjiva Lele, Stanford University
Intrepid Allocation: 12 Million Hours

Simulation of "High" Reynolds Number Turbulent Boundary Layers
Robert Moser, University of Texas at Austin
Intrepid Allocation: 33 Million Hours

Overcoming the Turbulent-Mixing Characterization Barrier to Green Energy and Propulsion Systems
Anurag Gupta, GE Global Research
Intrepid Allocation: 19 Million Hours

Lattice Gauge Theory

Lattice QCD
Paul Mackenzie, Fermilab
Intrepid Allocation: 67 Million Hours

Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations
Peter Coveney, University College London
Intrepid Allocation: 40 Million Hours

Quantum Simulations of Nanostructured Materials for Renewable Energy Applications
Giulia Galli, University of California—Davis
Intrepid Allocation: 1 Million Hours

Modeling the Rheological Properties of Concrete
William George, National Institute of Standards and Technology
Intrepid Allocation: 2 Million Hours

Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
Jeffrey Greeley, Argonne National Laboratory
Intrepid Allocation: 10 Million Hours

Electronic Structure Calculations of Nano Solar Cells
Lin-Wang Wang, Lawrence Berkeley National Laboratory
Intrepid Allocation: 1 Million Hours

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles
Christopher Wolverton, Northwestern University
Intrepid Allocation: 8 Million Hours

Nuclear Engineering

Predictions of Thermal Striping in Sodium-Cooled Reactors
Andrew Siegel, Argonne National Laboratory
Intrepid Allocation: 10 Million Hours

Nuclear Physics

Computational Nuclear Structure
David Dean, Oak Ridge National Laboratory
Intrepid Allocation: 15 Million Hours

Physics

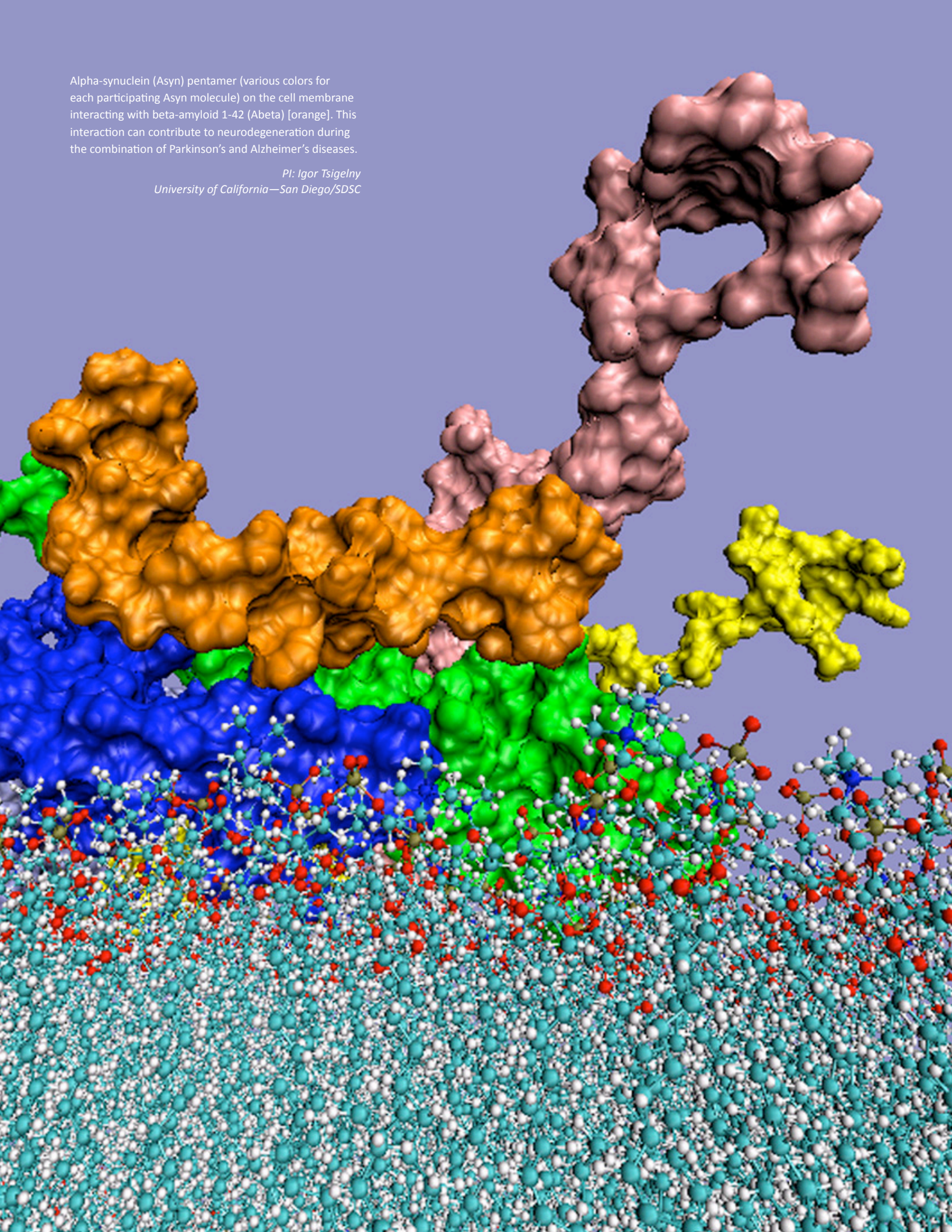
Unbalanced Magnetohydrodynamic Turbulence
Stanislav Boldyrev, University of Wisconsin—Madison
Intrepid Allocation: 25,000,000 Million Hours

Research into the Systematics of Type Ia Supernovae
Alan Calder, Stony Brook University
Intrepid Allocation: 35 Million Hours

Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond
Denise Hinkel, Lawrence Livermore National Laboratory
Intrepid Allocation: 45 Million Hours

Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models
Donald Lamb, The University of Chicago
Intrepid Allocation: 70 Million Hours

High-Resolution Global Simulation of Plasma Microturbulence
William Tang, Princeton Plasma Physics Laboratory
Intrepid Allocation: 12 Million Hours



Alpha-synuclein (Asyn) pentamer (various colors for each participating Asyn molecule) on the cell membrane interacting with beta-amyloid 1-42 (Abeta) [orange]. This interaction can contribute to neurodegeneration during the combination of Parkinson's and Alzheimer's diseases.

PI: Igor Tsigelny
University of California—San Diego/SDSC

APPENDIX A: "RESEARCH DISCOVERIES" IMAGE CAPTIONS

Page 18: Coolant-flow pressure distribution in a 217-pin wire-wrapped subassembly, computed on P=65536 processors of the Argonne Leadership Computing Facility's BG/P using Nek5000. The Reynolds number is Re~10500, based on hydraulic diameter. The mesh consists of 2.95 million spectral elements of order N=7 (~988 million gridpoints). The simulation pictured is a watershed computation, as it is the first to exceed one million elements (2.95 M used) and the first to use one billion gridpoints (0.988 B used).

Page 19: Four snapshots during a simulation of the explosion phase of the deflagration-to-detonation (DDT) model of nuclear-powered (Type Ia) supernovae. The images show extremely hot matter (ash or unburned fuel) and the surface of the star (green). Ignition of the nuclear flame was assumed to occur simultaneously at 63 points randomly distributed inside a 128-km sphere at the center of the white dwarf star. The images show volume renderings of extremely hot regions and the surface of the star [defined as the region in which the density is (1.0 - 1.25) x 10^{7} g cm^{-3}]. (a): 0.0 seconds, showing the initial distribution of ignition points. (b): 0.85 seconds, when the bubbles have become Rayleigh-Taylor unstable and developed into mushroom shapes on their way to the surface of the star. (c): 1.1 seconds, when the first plume of hot ash has made its way to the surface, and the flame front has entered the distributed burning regime, initiating a detonation. (d): 1.2 seconds, after several plumes of hot ash have reached the surface and multiple detonations have occurred, while the first detonation wave is propagating through the star. Images were created from a simulation run on the Blue Gene/P at the Argonne Leadership Computing Facility in 2009.

Page 20: Researchers determined this large protein, ALG13, which is 200 amino acids in length, with a new methodology called "NMR structure determination without side-chain assignments."

Page 22: Simulation of ventricular fibrillation (VF), a dangerous cardiac rhythm disorder, in a three-dimensional model of the canine ventricular anatomy.

Page 24: Alpha-synuclein pentamer on the membrane. The pentamer is constructed with theoretical docking of Asyn conformers that occur at 4 ns of MD simulation. These conformers have the best membrane contacting properties (calculated by the program MAPAS). The geometrical dimensions of this pentamer correspond to the experimentally elucidated by electron microscopy.

Page 25: A figure illustrating the peculiar electronic structure and three-fold coordination of the hydroxide anion (OH-) depicted in yellow surrounded by neighboring water molecules (depicted in red) in a configuration extracted from the vicinity of the air-water interface.

Page 26: This image represents a 3-D periodic mesoscale simulation of many small bubbles that exist during the early stages of foam formation. Results show that by using different surfactant structures, different bubble profiles can be produced. The blue mesh represents water, while surfactant molecules are represented by the white isosurfaces.

Page 27: Numerous controversies exist on the structural and dynamical properties of confined water. The image shown represents a non-polar surface.

Page 28: Total precipitable water, a measure of how much moisture is in the air, from December in a global simulation of the atmosphere at 1/8th of a degree. (Image credit: Jamison Daniel, ORNL National Center for Computational Sciences)

Page 29: For this flow, an important quantity called the potential enstrophy does not show any indication of organizing into two-dimensional structures, but rather remains three-dimensional at all scales in the flow.

Page 30: The figure shows a snapshot relative vorticity (in colors) and pressure (relief) at 100 m depth in a simulation with realistic, though idealized, forcing. Note the abundance of eddies away from the equator (at y = 0) and the large-scale separation between the smallest energetic features and the simulation domain. The color range spans ±5e-4 s{-1}. The domain is a simple “notched box” ocean with vertical walls and a periodic channel in the southernmost 1200 km.

Page 31: Pressure fluctuation (cylinder) and temperature iso-surface on a helicopter chamber demonstrator.

Page 33: Turbulent eddies are amplified upon passing through a shock wave. The flow is from left to right. The eddies are colored by their vorticity magnitude (rate of rotation); the shock is the dark thin sheet.

Page 34: Annular flow: liquid-vapor interface colored by local flow speed. High-speed vapor core drives vapor film to develop waves that break to produce drops and bubbles.

Page 35: This shows the 3-D structural model for Southern California and how the model is discretized for use in a simulation. (Image Credit: Geoffrey Ely, University of Southern California)

Page 36: The lattice QCD calculations performed of the decays and mixings of strongly interacting particles enable increasingly precise determinations of the parameters of the Standard Model of particle physics. This figure shows the bounds on the CP violating parameters rho and eta obtained from the mixings of K and B mesons with their antiparticles and from the decay of a B meson into a pion plus leptons.

Page 37: A nanoscale droplet of $Li_4BN_3H_{10}$, one of the configurations researchers are studying via *Ab-Initio* Molecular Dynamics to better understand the kinetics of hydrogen release in complex hydrides.

Page 38: The figure depicts a snapshot of blood flow simulated and visualised within a digitally reconstructed, patient-specific middle cerebral artery aneurysm. The top-left and top-right images show the volume rendering of the velocity field and of the stress respectively. The greyscale distribution shows blood pressure (bottom-left image) and stress (bottom-right image) at the inner surface of the aneurysm and surrounding blood vessels. The particle traces within the vasculature are colored according to the local velocity, effectively illustrating blood flow motion and portraying vortex fluid flow features.

Page 39: Snapshot from a molecular dynamics simulation of a system containing 16 isolated clay sheets immersed in a polymer melt. This system contains approximately 3 million atoms. The clay atoms are colored pink and brown; the polymer atoms are colored yellow.

Page 40: Part of a large comparison between 3-D time slices of a fluid in a weakly turbulent regime, with the goal of locating candidate suitable space-time orbits for the 4-D relaxation procedure. Darker regions signal less discrepancy between time slices for many different values of the period T. The system is a cubic lattice with L=64 and an ABC-force magnitude, simulated using the lattice Boltzmann method. The Reynolds number is 371.

Page 41: A CdSe/CdS core/shell nanorod calculated by the LS3DF code. Such nanorods have the potential to be used in solar cell applications. The green isosurface is the electron state, while the dark red isosurface is the hole. The CdSe core is located at the right-hand side, near the hole.

Page 42: A visualization of the flow of a complex suspension, concrete, with interactive controls.

Page 44: Three-dimensional structure of plasma microturbulence in a toroidal fusion device as calculated with a global gyrokinetic particle code developed at the Princeton Plasma Physics Laboratory.

Page 45: Electron density (blue) of a fast ignition target irradiated by an ultrahigh intensity laser (green-red) illustrating the occurrence of strong filamentation and the generation of a relativistic shock structure. Image generated from a simulation of the PIC code OSIRIS on Intrepid at the Argonne Leadership Computing Facility; Luís Silva, IST, Portugal; Warren Mori, UCLA.

Page 46: V. Rao Kotamarthi, Argonne National Laboratory, and his colleagues devised a new mathematical method to incorporate observational data into simulations more accurately and efficiently.

Page 47: Figure 1: The possible range of parameters that need to be investigated for evaluating the NH3-SO4-NO3 system.

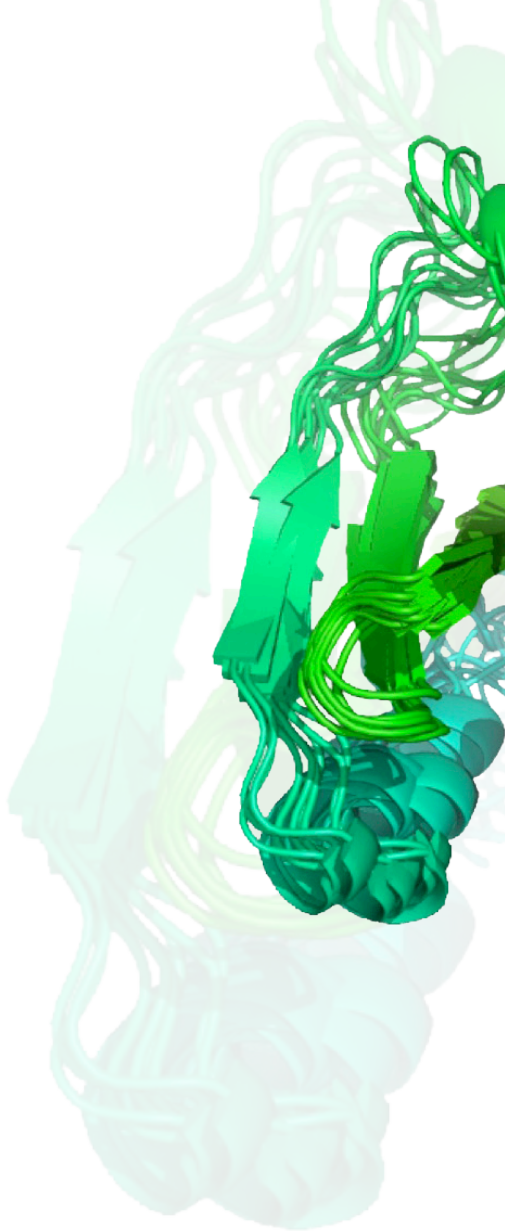
Page 47: Figure 2: Results from about 100 samples from a total of 500 simulations for ammonium nitrate in the coagulation mode. The Z axis shows the % deviation from the median at each altitude of the 500 simulations. The x-axis is the sample number, and the y-axis is the altitude in meters.

Page 48: High-fidelity capture of natural transition in the boundary layer demonstrated (within 1.5% x/c of measured value).

Page 49: Closeups of fracture simulations for nanocrystalline nickel without and with amorphous sulfide grain- boundary phases, where red, blue, and yellow colors represent nickel atoms inside grains (>0.5 nanometers from grain boundaries), nickel atoms within 0.5 nm from grain boundaries, and sulfur atoms, respectively. The figure shows a transition from ductile, transgranular tearing to brittle, intergranular cleavage. White arrows point to transgranular fracture surfaces.

ALCF STAFF

Expert staff helps researchers maximize ALCF resources and achieve the best applications performance, accelerating key scientific discoveries and engineering breakthroughs for humanity.



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U.S. DEPARTMENT OF ENERGY

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