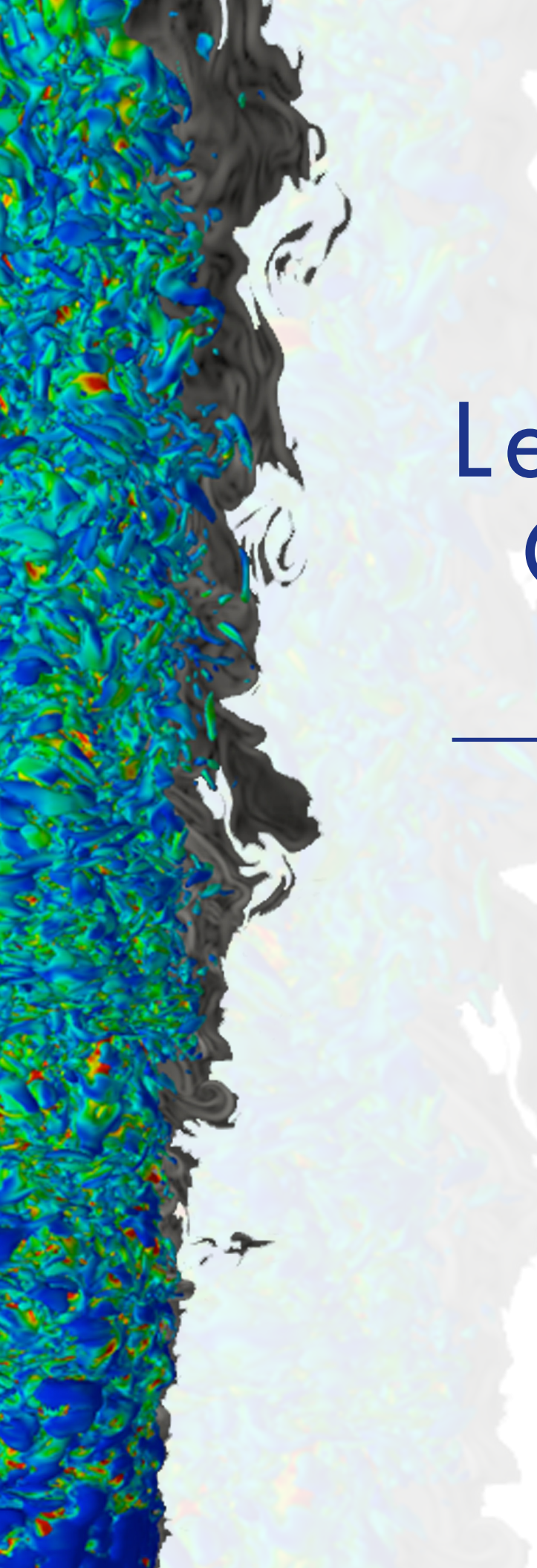

ANL-11/15

The Argonne Leadership Computing Facility

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

Argonne NATIONAL LABORATORY

Argonne Leadership Computing Facility

On the cover:
Turbulent structures in free shear layer flow from dual-flow conic nozzle–Vorticity contours plotted on constant Q surface. (Credit: Anurag Gupta/GE Global)

www.alcf.anl.gov
The Leadership Computing Facility Division operates the Argonne Leadership Computing Facility — the ALCF — as part of the U.S. Department of Energy's (DOE) effort to provide leadership-class computing resources to the scientific community.

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

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Director's Message

New Avenues for Science Powered by Supercomputing

Researchers found more ways than ever to conduct transformative science at the Argonne Leadership Computing Facility (ALCF) in 2010. Both familiar initiatives and innovative new programs at the ALCF are now serving a growing, global user community with a wide range of computing needs.

The Department of Energy's (DOE) INCITE Program remained vital in providing scientists with major allocations of leadership-class computing resources at the ALCF. For calendar year 2011, 35 projects were awarded 732 million supercomputer processor-hours for computationally intensive, large-scale research projects with the potential to significantly advance key areas in science and engineering. Argonne also continued to provide Director's Discretionary allocations — "start up" awards — for potential future INCITE projects. And DOE's new ASCR Leadership Computing (ALCC) Program allocated resources to 10 ALCF projects, with an emphasis on high-risk, high-payoff simulations directly related to the Department's energy mission, national emergencies, or for broadening the research community capable of using leadership computing resources.

While delivering more science today, we've also been laying a solid foundation for high performance computing in the future. After a successful DOE Lehman review, a contract was signed to deliver Mira, the next-generation Blue Gene/Q system, to the ALCF in 2012. The ALCF is working with the 16 projects that were selected for the Early Science Program (ESP) to enable them to be productive as soon as Mira is operational. Preproduction access to Mira will enable ESP projects to adapt their codes to its architecture and collaborate with ALCF staff in shaking down the new system. We expect the 10-petaflops system to stoke economic growth and improve U.S. competitiveness in key areas such as advancing clean energy and addressing global climate change.

Ultimately, we envision Mira as a stepping-stone to exascale-class computers that will be faster than petascale-class computers by a factor of a thousand. Pete Beckman, who served as the ALCF's Director for the past few years, has been named director of the newly created Exascale Technology and Computing Institute (ETCi). The institute will focus on developing exascale computing to extend scientific discovery and solve critical science and engineering problems. Just as Pete's leadership propelled the ALCF to great success, we know that that ETCi will benefit immensely from his expertise and experience. Without question, the future of supercomputing is certainly in good hands. I would like to thank Pete for all his effort over the past two years, during which he oversaw the establishing of ALCF2, the deployment of the Magellan project, increases in utilization, availability, and number of projects using ALCF1. He managed the rapid growth of ALCF staff and made the facility what it is today. All the staff and users are better for Pete's efforts.

Michael Papka

Pete Beckman

Michael E. Papka
Division Director (Interim)
Argonne Leadership Computing Facility
and Deputy Associate Laboratory Director
Computing, Environment, and Life Sciences
Argonne National Laboratory

Researchers worldwide use Intrepid, the IBM Blue Gene/P at the ALCF, to attack pressing problems in science at unprecedented scale and speed.

OVERVIEW

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

ALCF Provides the Science Community with Leadership-Class Computing Resources

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.

Research and Resources

Research endeavors are conducted at the ALCF through generous allocations of computer time and data storage awarded by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE), ASCR Leadership Computing Challenge (ALCC), Early Science, and Director's Discretionary programs.

Researchers who receive these allocations use one of the world's most powerful open-science supercomputers — the IBM Blue Gene/P system. Intrepid, the ALCF's 557-teraflops production machine, features 40,960 quad-core compute nodes; 163,840 processors; and 80 terabytes of memory, yet is highly energy efficient. The ALCF also operates Surveyor, a 4,096-core system used for tool and application porting, software testing and optimization, and systems software development. In addition, Eureka, a visualization supercomputer allows researchers to explore and visualize the flood of data they produce with Intrepid, and Gadzooks offers a test and development system for visualization.

User Support

ALCF catalysts, performance engineers, operations staff, and a data analytics and visualization team provide users with in-depth expertise and ongoing help in using the ALCF's computer systems. They provide users with information on ALCF services and resources, technical details on the IBM Blue Gene/P architecture, as well as hands-on assistance in porting and tuning applications. 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.

ALCF Leadership

Michael Papka

Pete Beckman

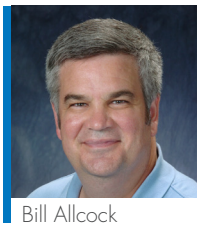
Laural Briggs

David Martin

Paul Messina

Kalyan Kumaran

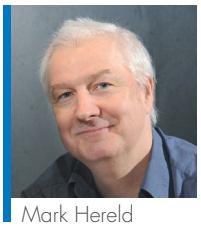
Susan Coghlan


Bill Allcock

Darin Wills

Katherine Riley

Ira Goldberg


Mark Hereld

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

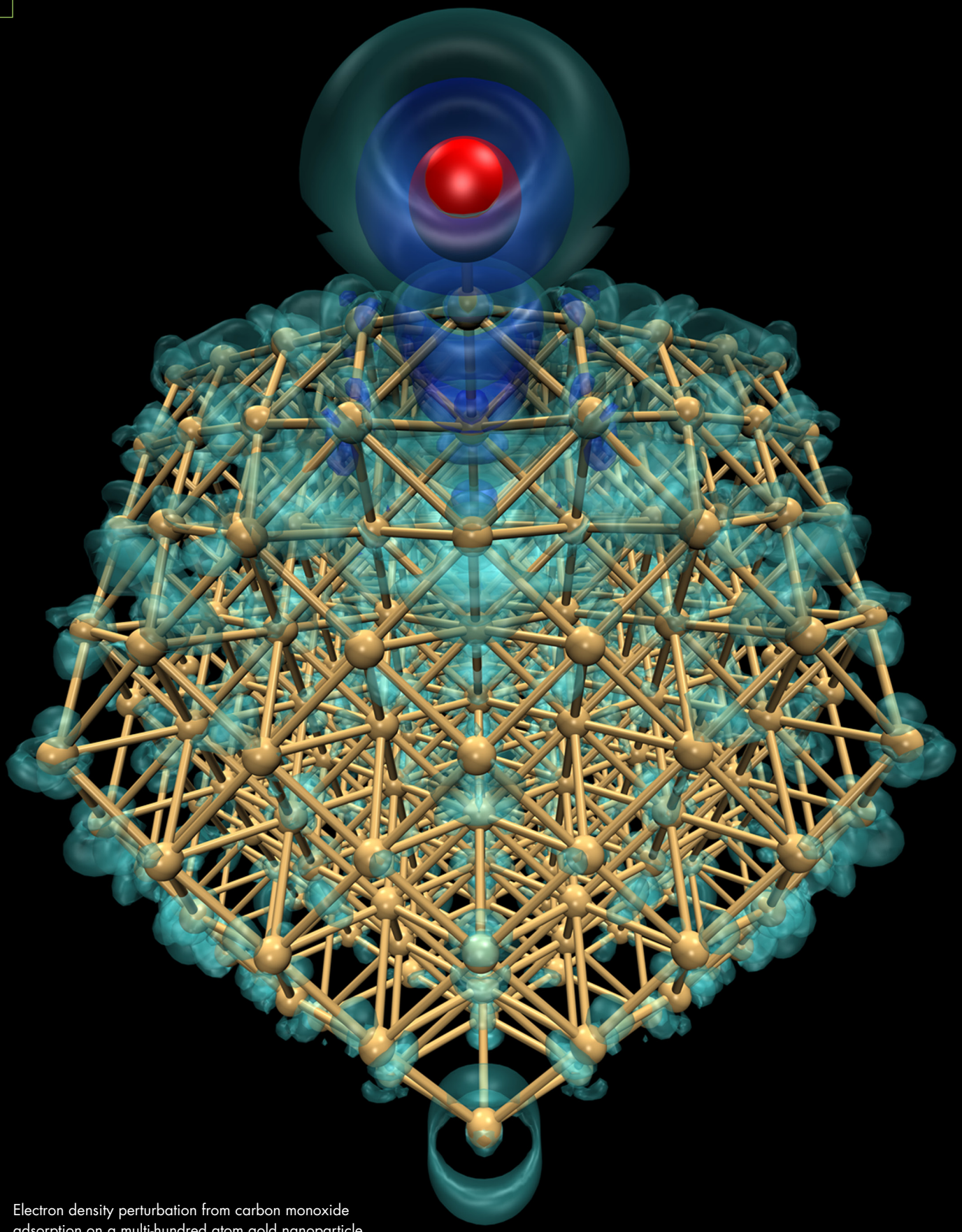
- Increased to 20 INCITE projects
- Began support of Early Science and INCITE projects on Blue Gene/P
- Dedicated the ALCF in April
- BG/P named world's fastest supercomputer for open science
- Installed Eureka, providing a quantum leap in visualization

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

2010

- Began support of 35 INCITE projects and 10 ALCC projects sponsored by the Department of Energy
- Signed contract for Mira, the next-generation Blue Gene/Q supercomputer
- Selected 16 Early Science projects to run on the 10-petaflops Mira
- Delivered more than 2 billion processor-hours of science



Electron density perturbation from carbon monoxide adsorption on a multi-hundred atom gold nanoparticle. The perturbation causes significant quantum size effects in CO catalysis on gold particles.

PI: Jeff Greeley/Argonne National Laboratory

SCIENCE HIGHLIGHTS

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

Science Director's Message

Intrepid Enables Advances in Diverse Science and Engineering Domains

Intrepid's powerful configuration hosts compute-intensive applications too large for previous systems, as well as providing an integrated environment for running ensembles of simulations that achieve breakthroughs in weeks or months, rather than years. ALCF staff's expertise in leading-edge computer systems and close interaction with users also contribute to the success of the projects. Consequently, usage has been high, as well as productive. In May 2010, less than two years after it entered production status, Intrepid's usage reached two billion core hours. The delivery of so many computing resources is certainly worth noting. However, far more important is the broad spectrum of scientific and engineering advances that resulted from the use of those hours.

For example, researchers are using Intrepid to:

- Design technologies to reduce aerodynamic noise and cut carbon emissions,
- Develop a new approach to protein mapping that requires much less experimental data and processing time,
- Assess the impacts of regional climate change,
- Gain insight into dangerous heart rhythm disorders,
- Identify the chemical cause of cracking in metals of interest in nuclear reactors, thus providing a way to make alloys so that cracking is less likely.

As scientific computing matures, scientists tackle ever more complex phenomena that require increasingly powerful resources. ALCF's next supercomputer, Mira, the 10-petaflops Blue Gene/Q system, is scheduled to be delivered in 2012. Mira will feature a peak speed four times greater than today's fastest supercomputer and nearly twenty times faster than Intrepid's, and larger memory and storage capacity.

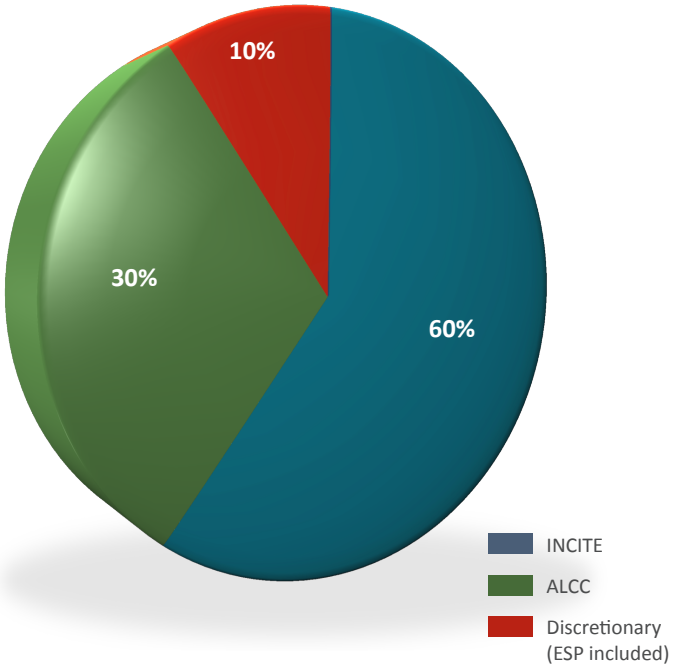
Take some time to browse through the science highlights in the following section.
We think you'll find the scientists' discoveries as compelling as we did.

Paul Messina
Director of Science
Argonne Leadership Computing Facility

From left to right: Pete Beckman, Director; Paul Messina, Director of Science; and David Martin, Manager of User Support and Outreach at the ALCF.

Forefront Computational Center in Extending Science Frontiers

Several initiatives enable bold research that ventures into unexplored science frontiers at the Argonne Leadership Computing Facility (ALCF). The Innovative and Novel Computational Impact on Theory and Experiment (INCITE), ASCR Leadership Computing Challenge (ALCC), Early Science, and Director's Discretionary programs all provide avenues for scientists to conduct breakthrough science and engineering.



Percentage of INCITE, ALCC, Director's Discretionary, and Early Science Program allocations at the ALCF.

Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program

ALCF resources are available to researchers as part of the U.S. Department of Energy's INCITE program. Established in 2003, the program encompasses high-end computing resources at Argonne and other national laboratories. The INCITE program specifically seeks computationally intensive, large-scale research projects with the potential to significantly advance key areas in science and engineering. The program encourages proposals from universities, other research institutions, and industry. It continues to expand, with current research applications in areas such as chemistry, combustion, astrophysics, genetics, materials science and turbulence.

ASCR Leadership Computing Challenge Program (ALCC)

Open to scientists from the research community in academia and industry, the ALCC program allocates resources to projects with an emphasis on high-risk, high-payoff simulations in areas directly related to the Department's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources. Projects are awarded an ALCC allocation based on a peer review for scientific merit and computational readiness.

Early Science Program (ESP)

Allocations through the Early Science Program (ESP) provide researchers with preproduction hours (between system installation and full production) on the ALCF's next-generation, 10-petaflops IBM Blue Gene system. This early science period provides projects with a significant head start for adapting to the new machine and access to substantial computational time. During this shakedown period, users assist in identifying the root causes of any system instabilities, and work with ALCF staff to help develop solutions. Three billion core hours are allocated through ESP.

Discretionary Projects

Discretionary allocations are "start up" awards made to potential future INCITE projects so that they can achieve computational readiness. Projects must demonstrate a need for leadership-class resources. Awards may be made year round to industry, academia, laboratories and others, and are usually between three and six months in duration. The size of the award varies based on the application and its readiness/ability to scale; awards are generally from the low tens of thousands to the low millions of hours.

Biological Sciences

How Do Researchers Predict the Structures of Biologically Important Proteins?

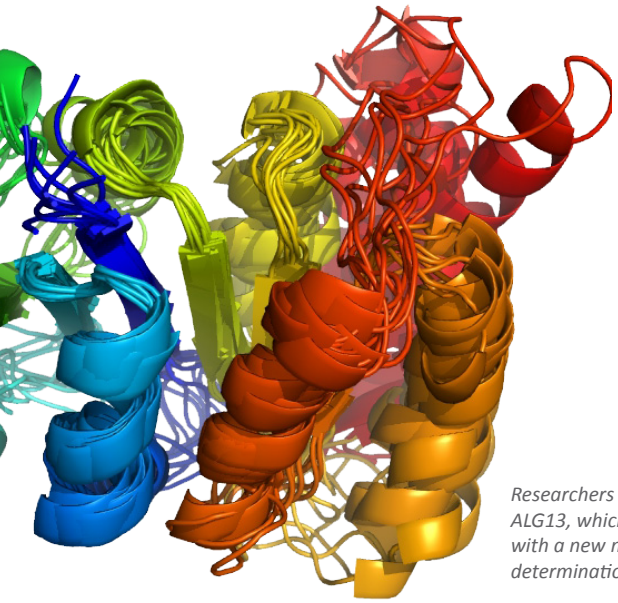
Principal Investigator: David Baker, University of Washington
INCITE Allocation: 50 Million Hours

Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires a detailed picture of their structure. Conventional protein structure determination using nuclear magnetic resonance (NMR) relies primarily on side-chain proton-proton distances. The necessary side-chain chemical shift assignment, however, is expensive and time-consuming, with possibilities for error. Moreover, approaches to NMR structure determination for larger proteins usually rely on extensive deuteration, which results in loss of key proton-proton distance information. Sparse structural data can be obtained from backbone-only experiments like orientational restraints from residual dipolar couplings and amid proton distances from NOESY spectra. These experiments are readily applicable even to fully deuterated and large proteins.

To determine NMR structures without side-chain chemical shift information, researchers incorporate backbone chemical shifts, residual dipolar couplings, and amide proton distances into the Rosetta high-resolution modeling methodology. To exploit the weak guidance signal provided by the sparse constraints, they developed an iterative scheme similar to a genetic optimization algorithm. A pool of the fittest individuals (e.g., lowest energy conformations) is maintained, and its worst part is replaced with offspring. The breeding or crossover of highly fit species (e.g., low energy conformations) is implemented as a Monte Carlo optimization that recombines features of previously found low-energy conformations. The type of features selected for recombination is adapted to the resolution of the pooled low-energy structures.

The iterative protocol increased the size range of accessible protein structures compared to the conventional Rosetta protocol. Researchers consistently solve protein structures up to 200 residues. Currently, they are determining the size range of this method and are testing further improvements. The INCITE program has been and will continue to be invaluable in its development.

Our INCITE work is focused on three areas currently. The first area is computing protein structures from very limited experimental data. With the INCITE computing resources, we are optimistic about developing methods which allow determination of the structures of proteins over 200 amino acids by NMR, which would be a big breakthrough in this area. The second area is designing proteins to bind very tightly to specific regions on a specified target. The third area is design of new enzyme catalysts. We are exploring catalysts for hydrogen production, solar capture, and other energy-related applications.



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."

Biological Sciences

Modeling the Molecular Basis of Parkinson's Disease

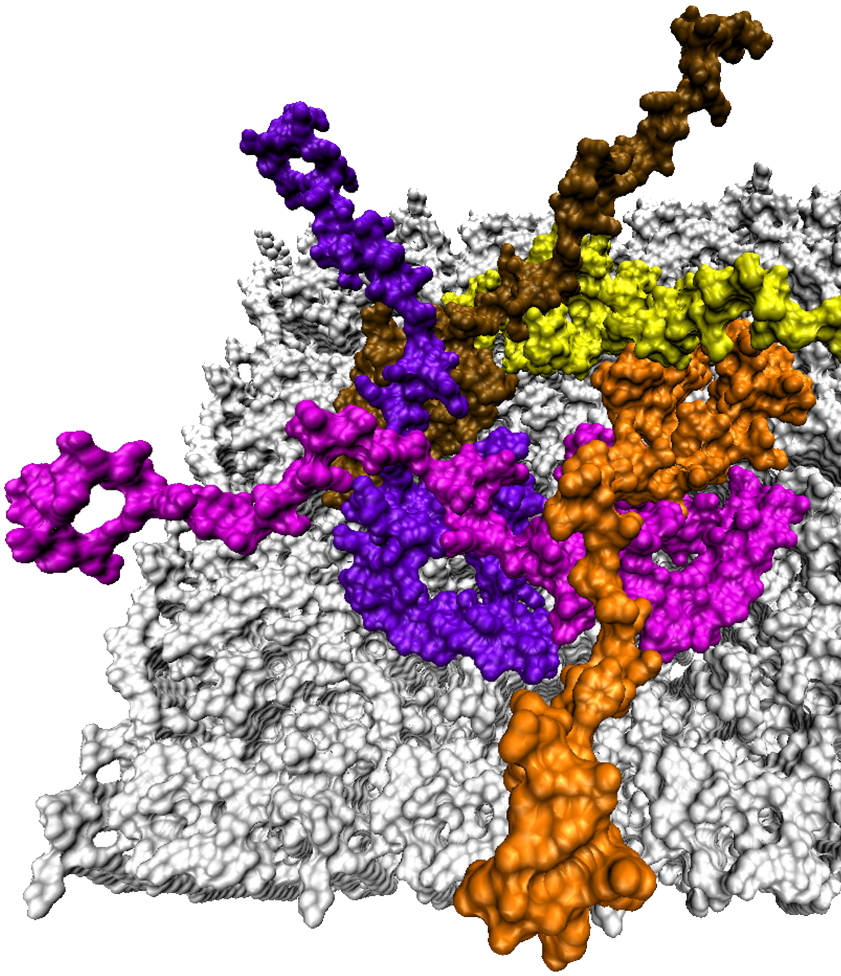
Principal Investigator: Igor Tsigelny | University of California–San Diego/SDSC
INCITE Allocation: 5 Million Hours

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

University of California–San Diego scientists 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 (ALCF) to learn more about the molecular basis of the disease and to explore ways to treat it. Scientists used alpha-synuclein in specific conformations as templates for possible pharmacophore hypotheses design. Such an approach made possible the design of drug candidates for the cure of Parkinson's disease.

Research is providing insights into the molecular mechanism for Parkinson's disease progression and will have broad applicability to other diseases. The findings also provide a test bed for identifying possible therapeutic interventions through computational modeling. Collaborator Dr. Eliezer Masliah and his laboratory are conducting experimental validation of the modeling and simulation results obtained. Given the encouraging correlation between the computational modeling predictions and laboratory experimental results, the team expects to make steady progress both with the computational model itself and with the design of effective drugs based on the computational modeling and simulations.

The research 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 of simulations being conducted and the scale of the simulations.



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.

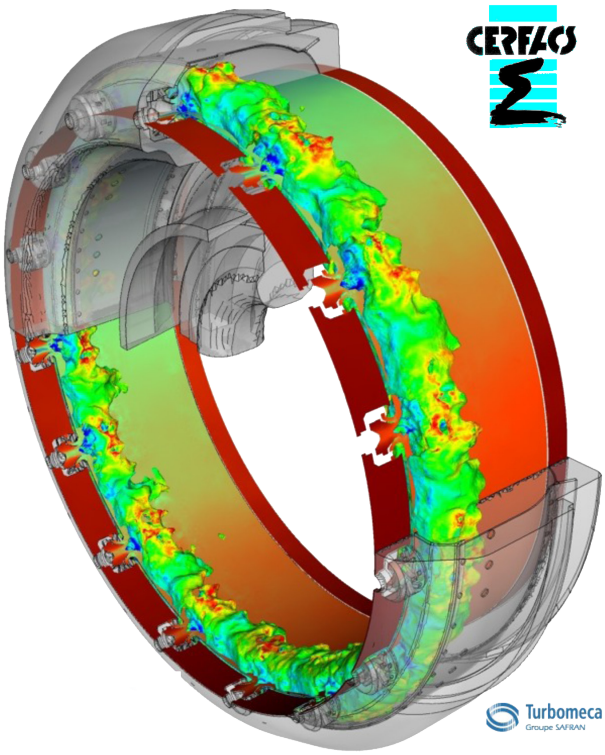
Chemistry

Performing the Largest Unstructured Large Eddy Simulation of a Real, Full Combustion Chamber

Principal Investigator: Thierry Poinsot, CERFACS
INCITE Allocation: 8 Million Hours

The increase of computer power has allowed science to make important strides in a variety of domains such as plasma studies, biomechanics, and molecular dynamics. With access to the INCITE program, researchers from CERFACS (the European Centre for Research and Advanced Training in Scientific Computation) have been able to perform top-of-the-line quality simulations on highly complex cases in their goal towards the fully numerical modeling of a real combustor.

This research is focused on Large Eddy Simulation (LES) of gas turbine engines with the inclusion of liquid phase phenomena. CERFACS has performed simulations and validation of two-phase flow experiments. In parallel, taking advantage of the leadership-class computer available at the Argonne Leadership Computing Facility, the researchers have performed the largest unstructured LES done to date of a real, full combustion chamber (330 million elements) on more than 16K cores. This simulation contributes to the validation of the LES approach when dealing with combustion instabilities. In these cases, the effects of mesh refinement are a highly critical point that was validated during the Stanford Center for Turbulence Research (CTR) summer program. A second mesh independency validation was performed, but this time it used a simpler, two-phase-flow single burner with three levels of refinement (4–, 8–, and 16–million elements). These results were published in the CTR Proceedings of the 2010 Summer Program by Cambridge University Press. Evaluation of the unbalance observed in Lagrangian simulations remains to be performed.



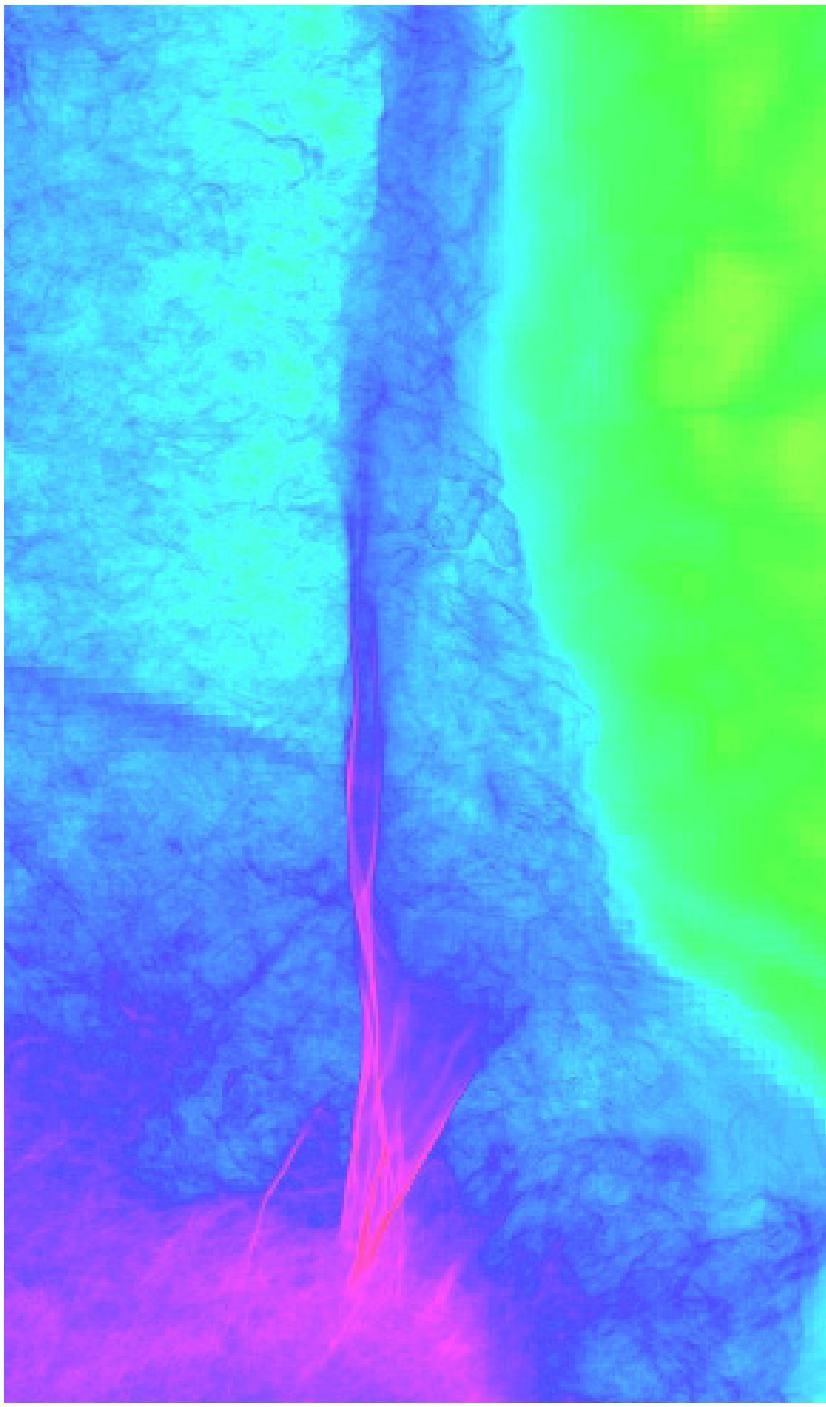
Fields of temperature and pressure in a simulation of a complete helicopter combustion chamber performed on the IBM Blue Gene/P at the ALCF (July 2010).

Combustion

High-Speed Combustion and Detonation (HSCD)

Principal Investigator: Alexei Khokhlov, The University of Chicago
Early Science Program Intrepid Allocation: 5 Million Hours

This project will gain insight into the physical mechanisms of the burning and detonation of hydrogen-oxygen mixtures. It will produce simulations to be used for the design of safe systems for future use of hydrogen fuel. The goal of the project is to create first-principles, petascale direct numerical simulation tools for understanding and predicting high-speed combustion and detonation (HSCD) phenomena in reactive gases. Researchers want to use first-principles simulations for fundamental understanding of the complex multi-scale physics of the transitory regimes of rapid flame acceleration and deflagration-to-detonation transition (DDT). The next-generation IBM Blue Gene system will enable them to perform first-principles simulations of DDT in a stoichiometric $2H_2 + O_2$ mixture initially at atmospheric pressure in a $100 \times 2.5 \times 2.5$ cm square tube. This is similar to a typical setup of the DDT experiments that measure run distances to detonation in reactive gases. Run distance is a critical parameter used for characterizing sensitivity of a reactive mixture to DDT, and it is used for assessing detonation hazard and designing severe accident mitigation strategies. In the experiments, burning is initiated by igniting a laminar flame in a quiescent gas near the closed end of the tube. As the flame expands, the turbulent boundary layer that forms near the tube walls increases the burning rate, and the flame accelerates rapidly. Secondary shocks and pressure waves generated inside the flame brush add to flame acceleration. Eventually, this leads to a localized explosion and the onset of a detonation wave.



Three-dimensional Navier-Stokes first-principles direct numerical simulation of a Mach=3 reflected shock bifurcation in a hydrogen-oxygen mixture in a square channel, performed within the high-speed combustion and detonation project (HSCD). Pseudo-schlieren image of a temperature field. Credits: Alexei Khokhlov (U of C), Charles Bacon (ANL), Shashi Aithal (ANL), Joanna Austin (UIUC).

Earth Science

A Proposal from the Geophysical Fluid Dynamics Laboratory to Perform Prototype Ultra High-Resolution Climate-Weather Modeling Studies at Argonne National Laboratory

Principal Investigator: Shian-Jiann Lin , Geophysical Fluid Dynamics Laboratory, NOAA
ALCC Allocation: 25 Million Hours

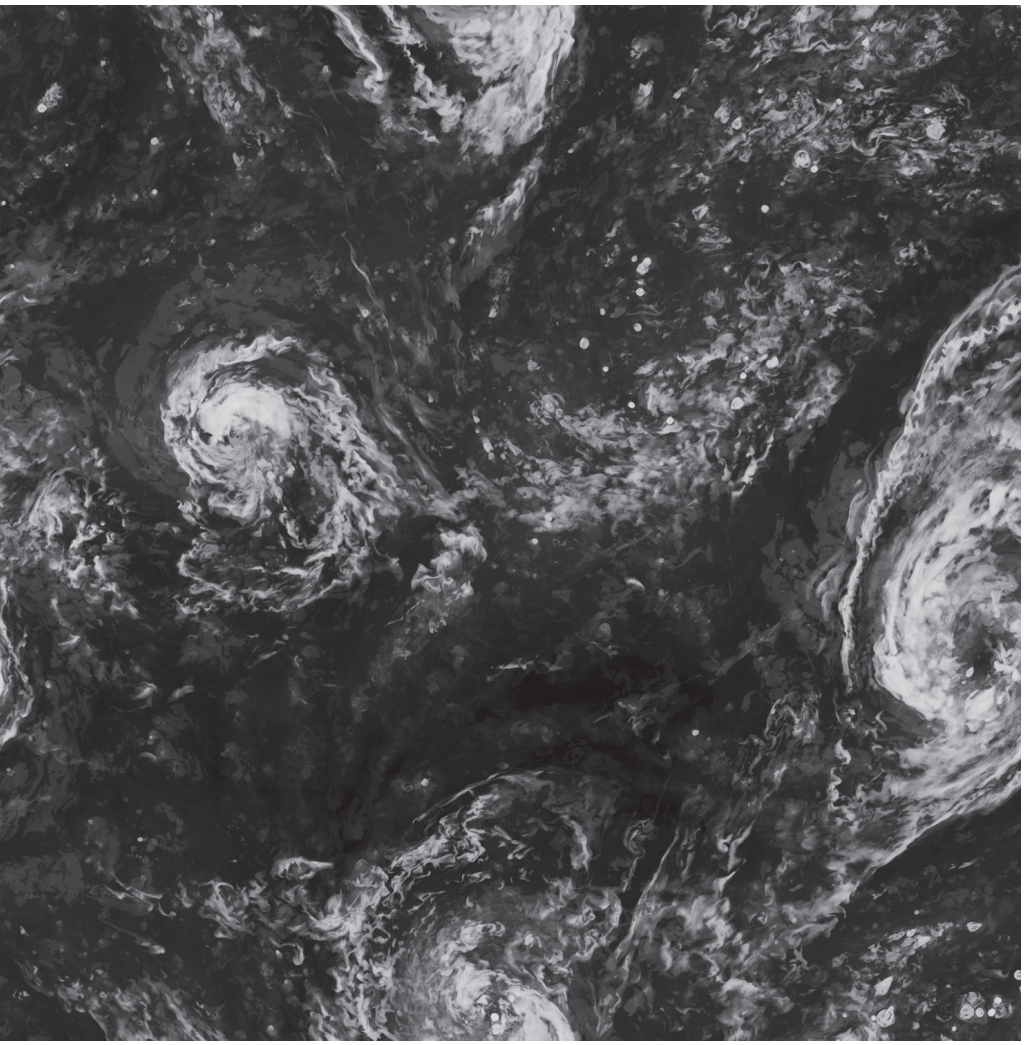
Researchers will explore the frontier of weather predictions and climate modeling with the newly developed Geophysical Fluid Dynamics Laboratory (GFDL) global cloud-resolving model with bulk micro-physics. In addition to validating the model with test cases, they will conduct three types of numerical experiments: (1) global simulations to validate 5-day hurricane forecasts during one hurricane season, (2) high-resolution global simulations of selected hurricanes, and (3) longer-term climate simulations.

The name of the GFDL code they will use is HIRAM. As a preliminary, they will validate the model's stability and dynamical formulation by running the standard Held-Suarez test case.

First, the researchers will run a set of hurricane hindcasts. For each of the 100 days of the 2008 Atlantic hurricane season, they will run a 12 km (average grid resolution) global hydrostatic simulation for 5 simulated days to produce a 5-day forecast. They will compare these to actual weather data for those 5 days. For each run, they will initialize using actual historical data for the starting day.

Second, the researchers will run ultra-high resolution 4.5 km non-hydrostatic simulations on five selected storms. They will focus on accuracy of hurricane track and intensity predictions.

Third, the researchers will run one-year high-resolution 12 km global simulations of the year 2008. This will be an ensemble of five Atmospheric Model Intercomparison Project (AMIP) style runs. They will document the simulated climate and severe weather events (such as hurricanes and typhoons) during this period.



Outgoing longwave radiation in the Doubly-Periodic Experiment, utilizing the Cubed-Sphere Non-hydrostaticAtmospheric Model (HIRAM) on an aqua-planet with a 5 km resolution. The research was conducted at the Geophysical Fluid Dynamics Laboratory, Princeton by Isaac Held, Shian-Jiann Lin, and Christopher Kerr.

Earth Science

How Can More Intricate Climate Models Help Curb Global Warming?

Warren Washington, National Center for Atmospheric Research
INCITE Allocation: 30 Million Hours

The effects of climate change are apparent in degrading air quality, intensified tropical storms, and the resulting destruction of coral reefs that protect the coasts from erosion and destructive waves. Global warming increases the occurrence of droughts, heat waves, wildfires, and floods. Scientists must improve the understanding of the impact of global warming so that society can optimally address climate adaptation considerations.

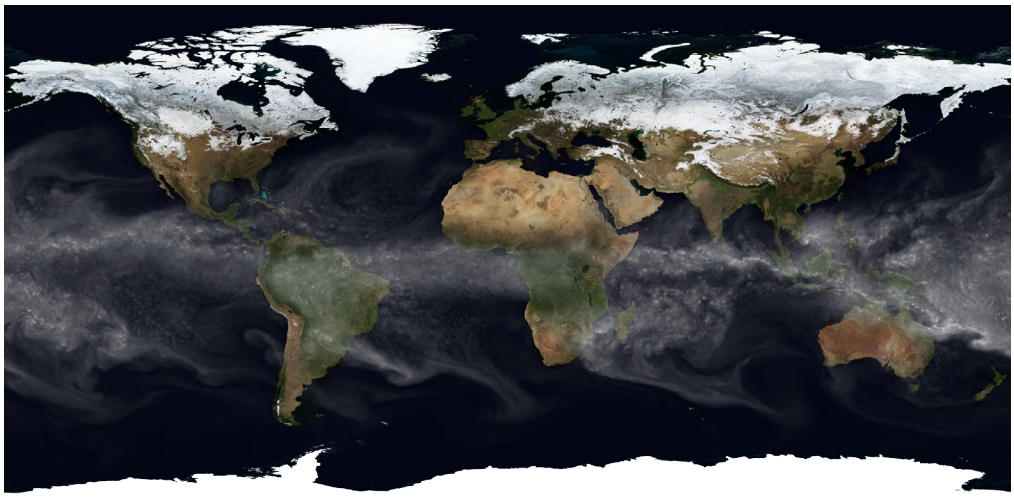
Advanced computation, like that possible on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF), allows researchers at the DOE laboratories and National Center for Atmospheric Research (NCAR) to develop more complex and intricate climate models. The vital information these improved models provide will help guide environmental policy.

The Department of Energy awards allocations of computing resources for climate studies across multiple laboratories through the INCITE program. In turn, the Climate Science Computational End Station (CCES) organizes and coordinates these computational efforts.

Using ALCF resources, CCES is advancing climate science through both aggressive model development activity and an extensive suite of climate simulations to correctly simulate the global carbon cycle and its feedback to the climate system, including its variability and modulation by ocean and land ecosystems.

Researchers are testing a new, highly scalable method for solving the fluid dynamics of the atmosphere for use in future climate simulations. This model, called HOMME, has run with a resolution as high as 1/8th of a degree of latitude on more than 80,000 cores.

Next, researchers will use HOMME to perform standard climate model benchmark simulations for comparisons with other models. They will also test the new version of the Community Earth System Model on the ALCF's Blue Gene/P.



Total precipitable water, a measure of how much moisture is in the air from a single moment in time in the global simulation of the atmosphere at a resolution of half a degree of latitude. (Figure provided by Mark Taylor, Sandia National Laboratories.)

Energy Technologies

Materials Design from First Principles

Principal Investigator: Larry A. Curtiss, Argonne National Laboratory
ALCC Allocation: 20 Million Hours

New materials may help solve global energy challenges

Our energy future hinges on the design and discovery of new materials — like materials to replace the oils currently used to make plastics and materials to power electric vehicles.

Scientists at Argonne's Center for Nanoscale Materials are pairing the power of the ALCF's Blue Gene/P with newly available electronic structure codes to conduct massively parallel quantum chemical calculations for use in the design of breakthrough materials that may have energy-related applications.

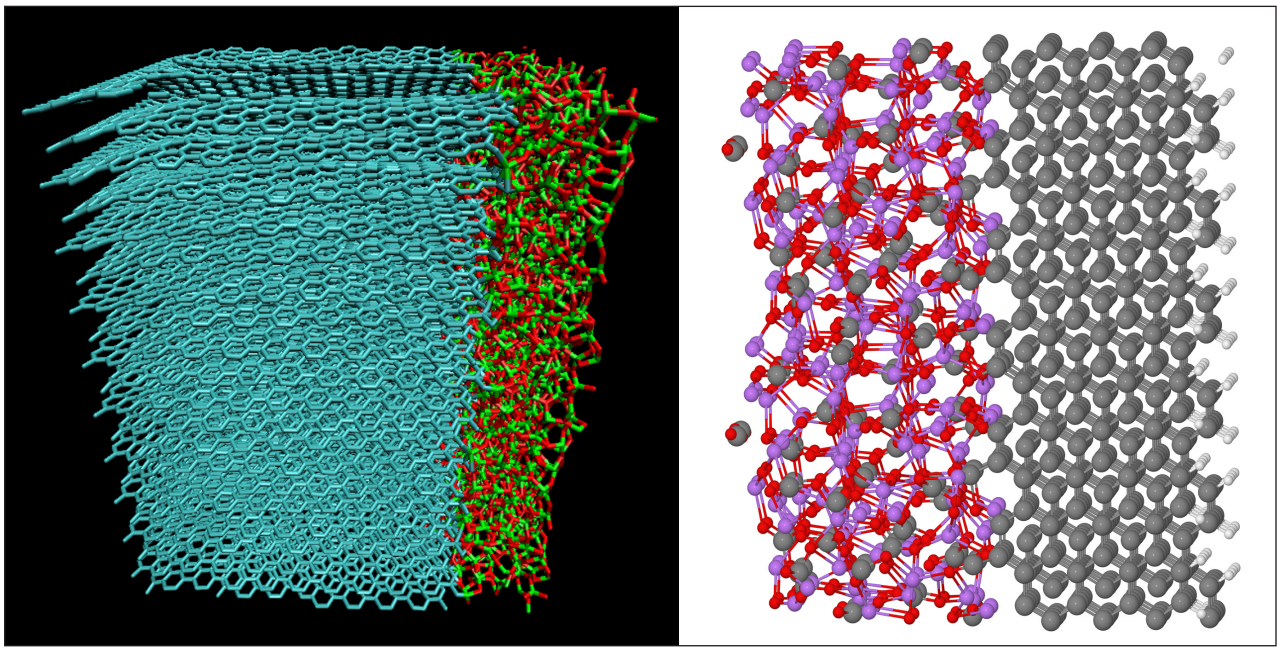
Materials reduce greenhouse gases, power electric vehicles

Research efforts will focus on catalytic materials and materials used for electric energy storage. Catalytic materials are used for bond-specific activation for efficient chemical transformations. This research could yield new strategies for more energy-efficient, environmentally friendly chemical synthesis to help reduce greenhouse gases, or in new methods for replacing petrochemicals with inexpensive, abundant small alkanes.

Creating new materials for electrical energy storage (specifically, for the interface between electrolyte and electrode) could lead to safer, longer-range batteries for electric vehicles.

Finding better solutions faster

With models of surfaces and interfaces in materials created from first-principles calculations not previously possible, scientists can conduct large-scale screening using a Materials Design Workbench developed at Argonne. Researchers will employ GPAW and NWCHEM codes adapted for massively parallel machines like the Blue Gene/P. Screening allows the scientists to focus efforts on the most promising materials.



Models for the solid electrolyte interphase in Li batteries: Amorphous alumina on graphite (left) and Li_2CO_3 on graphite (right).

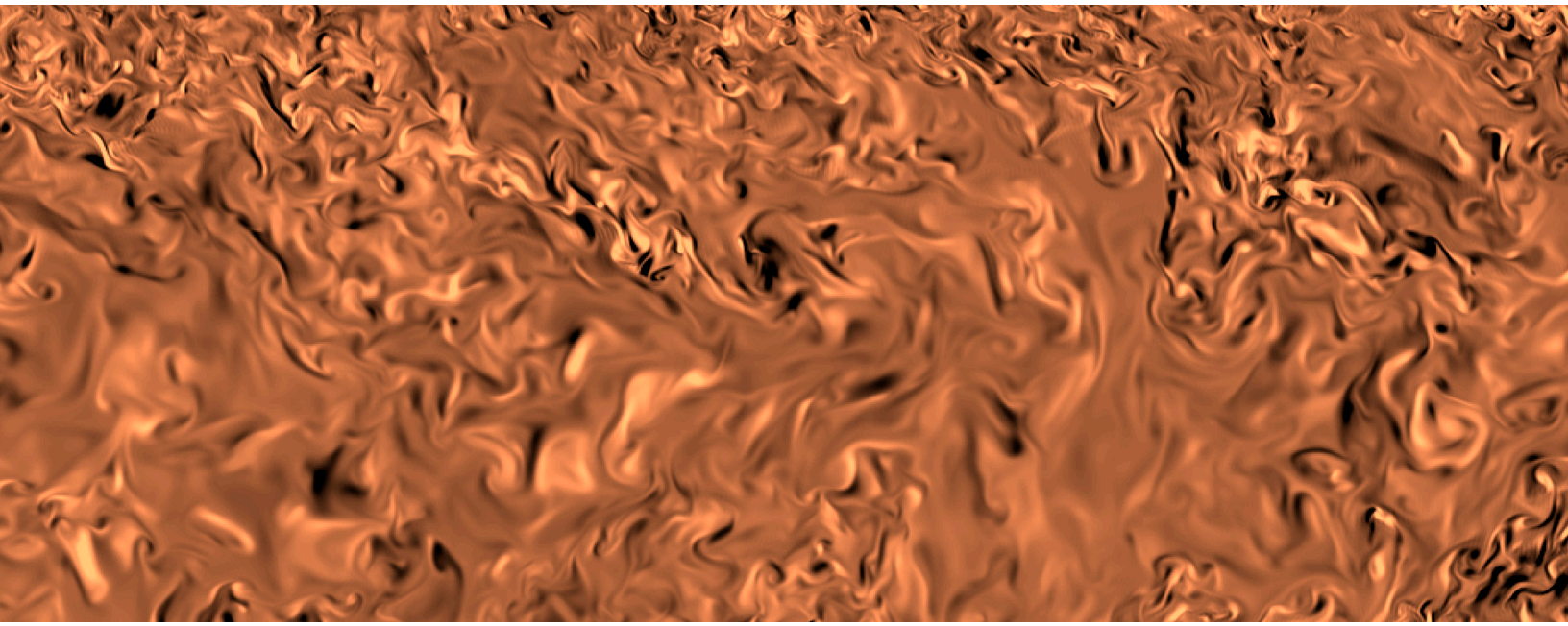
Energy Technologies

Petascale Direct Numerical Simulations of Turbulent Channel Flow

Principal Investigator: Robert Moser, University of Texas
Early Science Program Intrepid Allocation: 5 Million Hours

Researchers propose to use the petascale computing power of the next-generation Blue Gene system to perform direct numerical simulations (DNS) of high Reynolds number turbulent wall-bounded flow in a channel. This DNS is aimed at developing a nearly complete understanding of the phenomena dominating wall-bounded turbulence, which is central to the energy losses inherent in transportation. The impact of such a development will likely be profound. Approximately 28% of U.S. energy consumption is expended on transportation. This energy expenditure is due to the interaction between solid surfaces (of vehicles or pipes) and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. Since much of the drag in these flows is due to turbulent skin friction, much of this energy consumption results from wall-bounded turbulent shear layers.

The central emphasis of this research is on reaching a sufficiently high Reynolds number to explore the physics that arise in the overlap region. The overlap region is where the viscous near-wall turbulence interacts with the outer-layer turbulences. This interaction is key to understanding high Reynolds number turbulent wall layers. To investigate this interaction, it is necessary that the Reynolds number be sufficiently high so that there is a substantial disparity in scale between the inner and outer layers. The results can then be extrapolated to arbitrary Reynolds numbers. This simulation will be performed using the supercomputing software that the proposing team has developed and benchmarked on Blue Gene/P and will further optimize for performance on the next-generation Blue Gene.



Spanwise vorticity in a turbulent channel flow at Re_tau=2000. This is the current highest Reynolds number for the flow, simulated by collaborator Javier Jimenez and his colleague, Sergio Hoyas. The Early Science project will perform a simulation at Re_tau=5000, which will allow researchers to address a number of questions regarding the High Re wall-bounded turbulence that is not possible at the lower Re.

Engineering

A Center for Turbulence Research — Argonne Leadership Computing Facility Collaboratory for Very Large Scale Turbulence Simulations on Petascale Computing Platforms

Principal Investigator: Parviz Moin, Center for Turbulence Research, Stanford University
ALCC Allocation: 50 Million Hours

New turbulence collaboration enhances energy security

The Center for Turbulence Research (CTR) and the Argonne Leadership Computing Facility (ALCF) have joined forces to enhance the state of the art of turbulence simulations by harnessing the computing power of the Blue Gene/P via allocations from the ASCR Leadership Computing Challenge (ALCC) program.

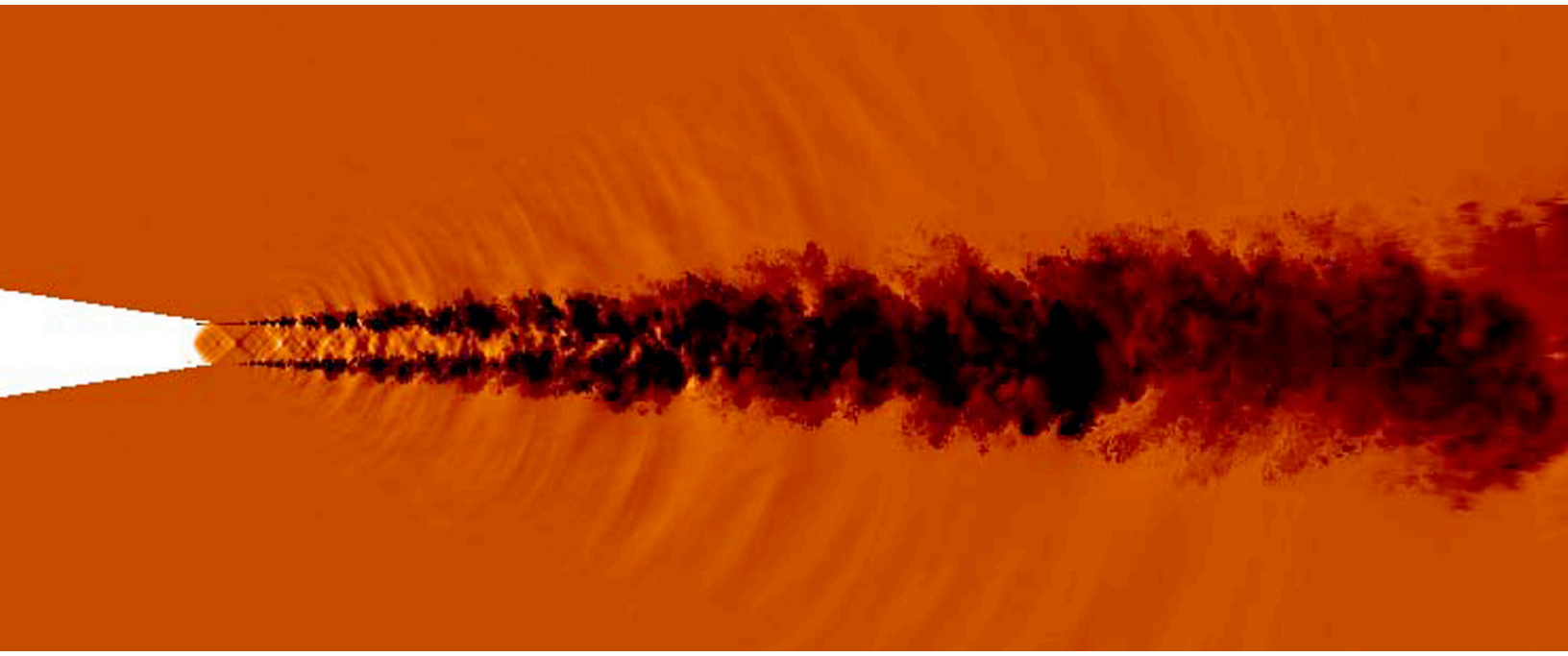
The collaboration will focus on high-risk, high-payoff turbulence simulations linked to advancing national energy security, including studies of aerodynamic noise reduction in next-generation aircraft propulsion systems, heat transfer in advanced energy systems, and related simulations.

Reducing jet engine noise

Initially, the CTR-ALCF collaboration will study the effects of chevrons on turbulent mixing of jet engine exhaust streams and on the role chevrons play in noise suppression. Chevrons — serrated geometric edges installed on aircraft engines — greatly reduce noise by mixing exhaust jet streams. Their design, however, must balance their role in reducing noise with performance reductions they might cause.

New simulations aim to tell the full story

To date, most simulations model the effects of chevrons by source-and-sink terms in the governing equations rather than by resolving their complex, small-scale geometric details. The proposed simulations aim to fully resolve the effects of the chevrons in a jet engine to capture the enhanced shear layer mixing the chevrons generate and, in turn, to evaluate possible noise-mitigation strategies.



Simulation of an expanding supersonic jet and the radiated acoustic field.

Engineering

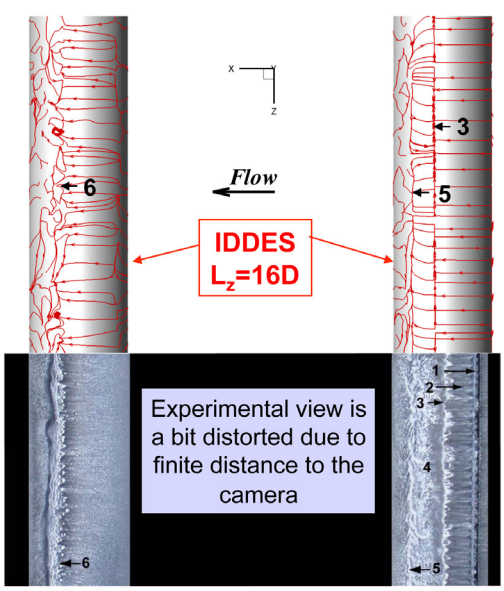
Employing Improved Delayed Detached Eddy Simulations for Turbulent Flows over Tandem Cylinders

Principal Investigator: Philippe Spalart, Boeing

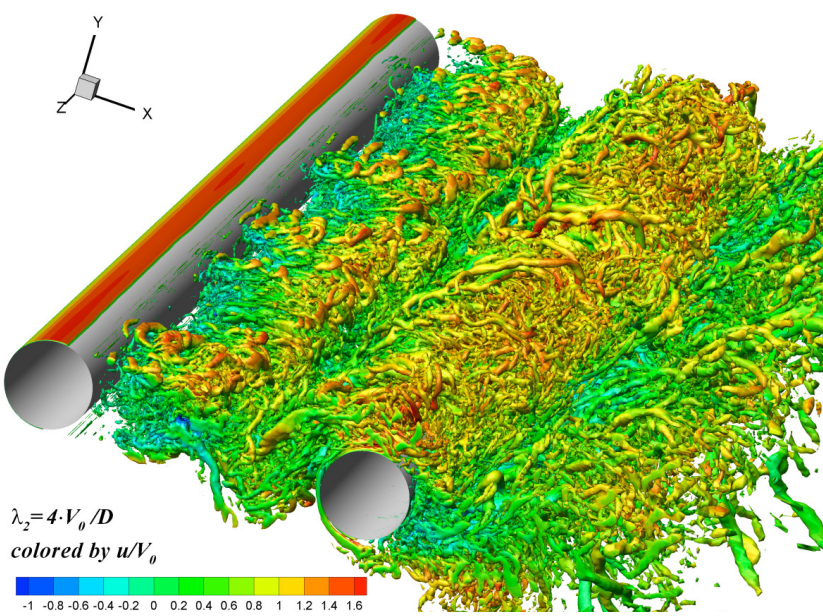
Director's Discretionary Allocation: 11 Million Hours

The flow past Tandem Cylinders is a prime test case for detailed comparisons between CFD and experiments, with particular focus on the physics of massively separated flows, the impingement of turbulence on a solid body, and the noise that results from this interaction. Such flow scenarios occur in a wide variety of applications that include (but are not limited to) aircraft landing gear, wind turbines, bridges, industrial heat exchangers, and a myriad of architectural situations. Very recently, researchers from Boeing and NTS (St. Petersburg, Russia) have computed, on the IBM Blue Gene/P at the Argonne Leadership Computing Facility, massively separated flows over tandem cylinders using a novel algorithm known as the Delayed Detached Eddy Simulation (DDES) and its variant, the Improved Delayed Detached Eddy Simulation (IDDES). This new approach to computing turbulent flows creatively blends Reynolds Averaged Navier-Stokes (RANS) computations in the near wall region (i.e., at the surface of the cylinder) with Large Eddy Simulation (LES) computations in regions away from the wall. The tandem cylinder simulations on the Blue Gene/P are among the largest, with a computational domain spanning sixteen diameters in the cross-flow direction. Experiments done at NASA Langley indicate that at this span-wise length, the lateral pressure and velocity correlations begin to approach zero, thereby justifying the periodic boundary conditions used in the numerical simulations.

The NTS code, that has been used for the simulations, is a structured, multiblock, overlapping grid, finite volume code. The range of numerical schemes implemented in the code includes implicit high order hybrid (weighted 5th order upwind/4th order centered) flux difference splitting schemes of Rogers and Kwak for incompressible flows and of Roe for compressible flows. Numerical implementation of these schemes is performed by implicit relaxation algorithms (Plane/Line Gauss-Seidel relaxation and Diagonally Dominant ADI algorithm), which may be arbitrarily specified by a user in different grid-blocks. In addition, the code is capable of running in hybrid (i.e., MPI+OpenMP) mode and shows very good weak scaling on the Blue Gene/P.



Comparison of oil-flow patterns from DDES at Lz=16D with experiment: 1-transition strip; 2-streaks from streamwise vortices generated by transition strip; 3-primary separation line; 4-spanwise flow between 2 separation lines; 5-secondary separation line; 6-rear cylinder separation.



Isosurface of swirl λ=4.0V0/D for Lz=3D and Lz=16D.

Lattice Gauge Theory

How Can We Better Understand the Basic Building Blocks of Nature?

Principal Investigator: Paul Mackenzie, Fermilab
INCITE Allocation: 67 Million Hours

Scientists have long sought to understand the basic building blocks of nature. While the behavior of particles such as protons and neutrons is well understood, less is known about the interactions of quarks and gluons, which compose them, the even-smaller particles that make up protons and neutrons. Because they interact very differently than larger particles, the study of interactions between quarks and gluons, Quantum Chromodynamics (QCD), requires different methodology. With the help of supercomputers, scientists use a four-dimensional lattice representation of space-time to analyze QCD.

This research aims to deepen the understanding of the interactions of quarks and gluons, the basic constituents of 99 percent of the visible matter in the universe. It will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature.

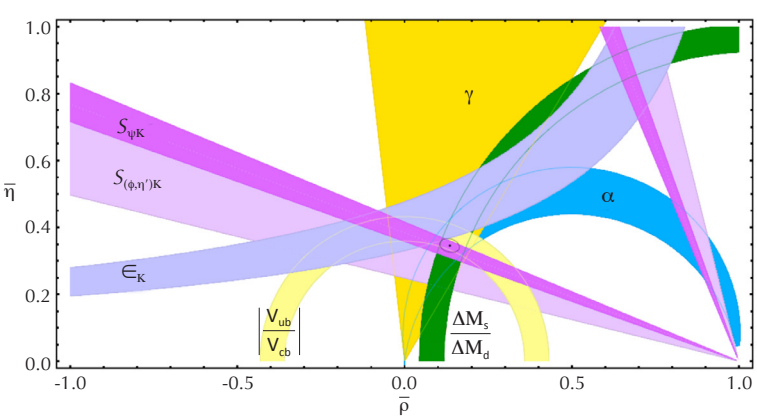
Scientists conducting QCD research have logged over 300 million core hours on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF). The scientists have generated gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to their physical values found in nature. The gauge configurations are being used 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 previously possible with other machines.

Domain-wall configuration ensembles of lattice spacings 0.114 femtometers (fm) and 0.086 fm have been completed on lattices of sizes $24^3 \times 64$ and $32^3 \times 64$, respectively. These are the largest domain-wall lattices ever attempted. For the staggered quarks, a set of runs with a lattice spacing of 0.06 and 0.045 fm have been completed. These are the most challenging staggered ensembles generated to date.

These ensembles are currently being analyzed at the ALCF and elsewhere 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. These calculations are enabling precise tests of the Standard Model, aiding in a deeper understanding of fundamental physics.

Improved versions of both methods for lattice fermions are under way. For domain-wall fermions, a new method has been developed (the "AuxDet" method) that will permit a closer approach to the physical, light quark limit. For staggered fermions, an improved discretization method has been developed ("hisq" fermions) that substantially reduces discretization errors. New ensembles with the improved methods are expected soon.



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.*

Materials Science

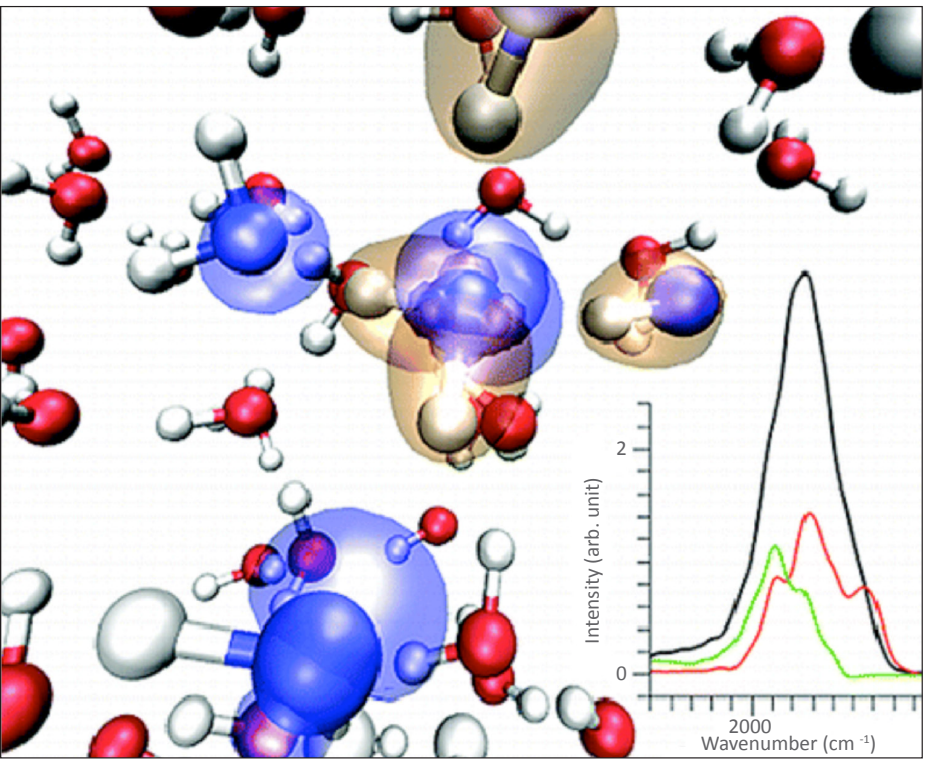
Interpreting IR Stretching Band of Liquid Water Improves Understanding of Hydrogen Bonding

Principal Investigator: Giulia Galli, University of California–Davis
INCITE Allocation: 1 Million Hours

In the last several decades, vibrational spectroscopy has been widely used to probe the structure and dynamics of water, and much progress has been made in the understanding of hydrogen bonding in the liquid, based on two-dimensional (2-D) IR spectroscopy. However, despite experimental and theoretical advances (e.g., the interpretation of IR and 2-D-IR spectra provided by several simulation studies), a detailed understanding of the infrared (IR) line shapes of liquid water has not yet been achieved.

University of California–Davis researchers interpreted the complex shape of the IR stretching band of neat, heavy water, using first principles molecular dynamics and *ab-initio* electronic structure calculations. They carried out calculations using the Qbox code on Intrepid, the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility. The researchers showed that intermolecular dipolar correlations play a key role in determining the shape and width of the band, and that these correlations are long-ranged, extending to the second coordination shell. Both hydrogen-bonded and non-hydrogen-bonded molecules contribute to the IR stretching band over the entire frequency range, with no distinctive peak or shoulder associated with each species. Within a molecular orbital picture, the researchers identified specific features of the band arising from correlations of electronic contributions to the IR activity. The researchers' interpretation of the IR stretching band of water is providing a better understanding of hydrogen bonding. Additional spectroscopic investigations carried out by the UCD team, in collaboration with researchers at LLNL and MIT include the study of X-Ray absorption spectra.

Physics issues that remain to be explored include the effects of the presence of solvated ions on the properties of neat and confined water and the analysis of electronic spectra (e.g., x-ray absorption spectra).



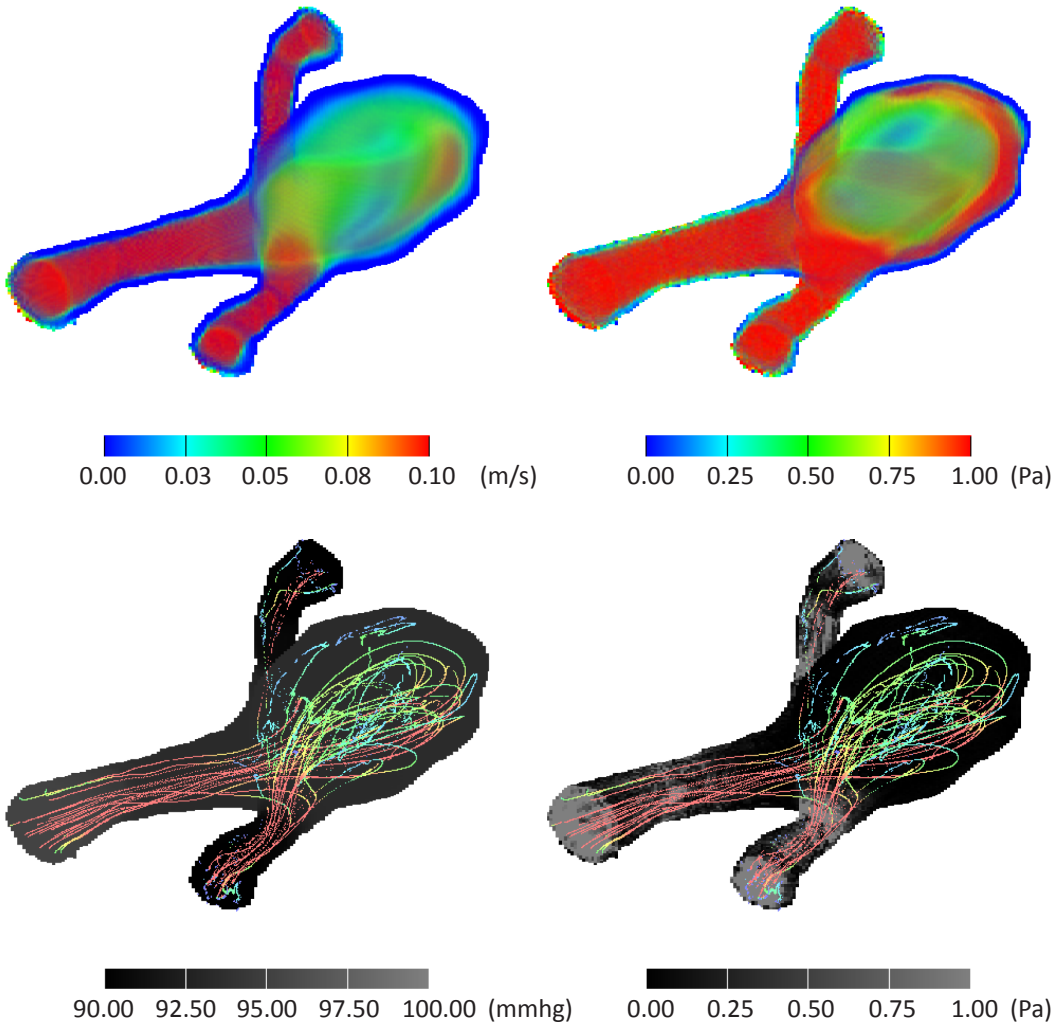
Molecular orbital representation of the electronic states in the first solvation shell in water. The inset shows different contributions (total, inter- and intra-molecular) to the IR stretching band of liquid water.

Materials Science

Large-Scale Condensed Matter and Fluid Dynamics Simulations

Principal Investigator: Peter Coveney, University College London
INCITE Allocation: 40 Million Hours

Patient-specific brain blood flow simulations are aiming to improve diagnosis and treatment of aneurisms. Researchers from University College London have made significant progress in studying three patients' internal carotid artery aneurysms. In conducting the simulations, the researchers used HemeLB, a sparse-geometry optimized lattice Boltzmann code, on Intrepid, the 557-teraflops IBM Blue Gene/P, at the Argonne Leadership Computing Facility. Intrepid allows flow calculation at speeds fast enough to be clinically useful. The simulations involved a number of steps — acquiring angiography data, transferring it to local resources, pre-processing locally, staging to remote resources for simulation, and reporting (using interactive steering and visualization).



A visualization of one aneurysm. Top Left: volume rendered velocity. Top Right: volume-rendered von Mises stress. Bottom Left: external pressure and streaklines. Bottom Right: external von Mises stress and streaklines.

Materials Science

Probing the Non-scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

Principal Investigator: Jeff Greeley, Argonne National Laboratory

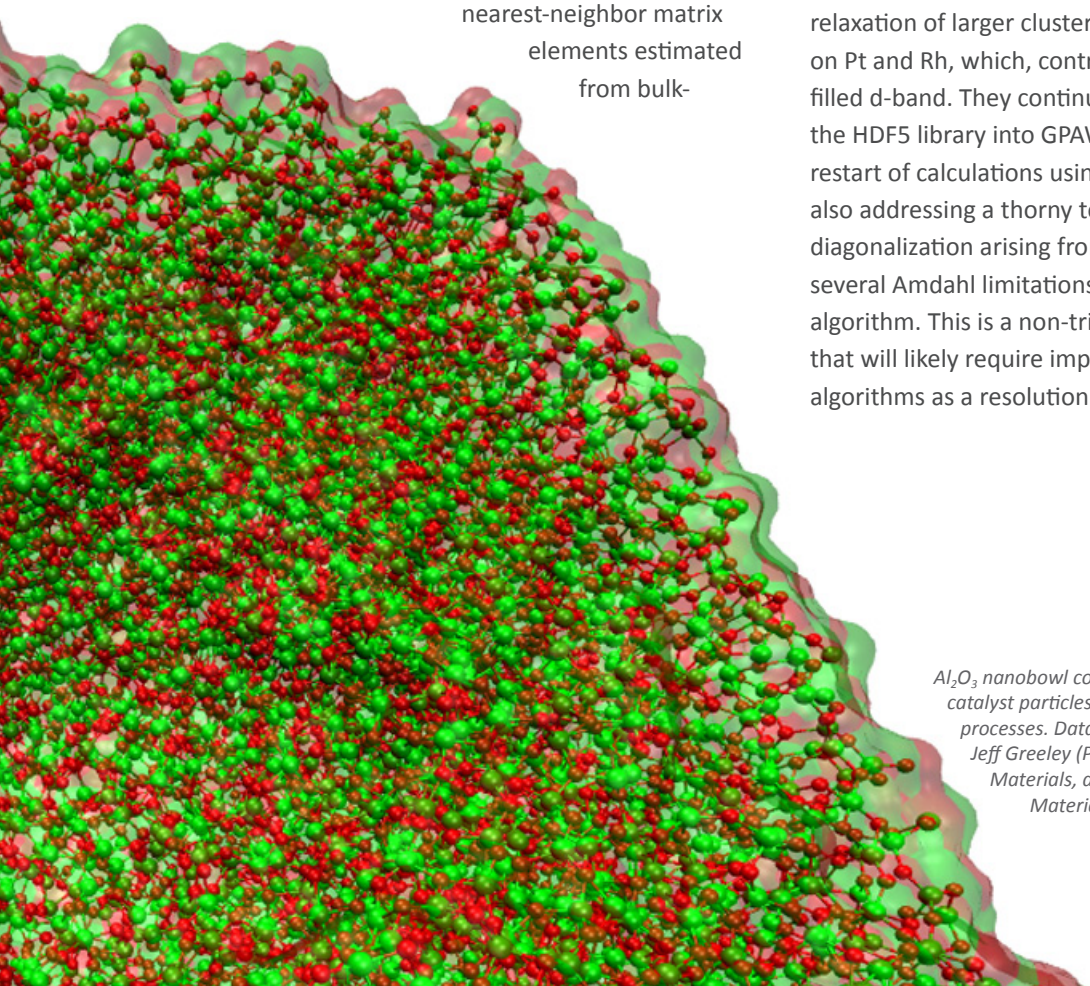
INCITE Allocation: 10 Million Hours

To get insight into quantum-size effects (QSE) of nano-clusters and estimate the impact on their catalytic ability, Argonne researchers, in collaboration with colleagues at the Technical University of Denmark, performed Density Functional Theory (DFT) calculations on cuboctahedral gold clusters with adsorbed oxygen and carbon monoxide. The effective cluster sizes ranged from 0.5 to about 4 nm (13 to 1,415 atoms). The calculations were done on the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility. The researchers found the QSE to be energetically converged for clusters larger than 309 atoms — where they obtained the adsorption characteristics of single crystal surfaces. The QSE effects were on the order of 1 eV and had a huge impact on the estimated catalytic properties of the clusters. They also found the QSE to be essentially reproduced by a simple, tight-binding model with nearest-neighbor matrix elements estimated from bulk-gold calculations and fit to reproduce the adsorption characteristic of the single-crystal surfaces.

Research accomplishments include:

- Completed parallelization of dense linear algebra — can now always run in VN mode with state-parallelization and will never run out of memory;
- Found new, efficient BG/P mappings;
- Did additional general tuning of the parallel performance and are working more closely with IBM to optimize the code further;
- Discovered a scheme that corrects for numerical grid effects (egg-box effect), which can sum up to several eVs for large systems — and which furthermore influence the relaxation of clusters (grid-snapping to hotspots of the egg-box effect).

Currently, the researchers are pursuing geometric relaxation of larger clusters and focusing their efforts on Pt and Rh, which, contrary to Au, have a partially filled d-band. They continue to work on integrating the HDF5 library into GPAW to allow the efficient restart of calculations using wave functions. They're also addressing a thorny technical challenge: Dense diagonalization arising from ScaLAPACK is one of several Amdahl limitations in the canonical O(N3) DFT algorithm. This is a non-trivial algorithmic bottleneck that will likely require implementing O(N) DFT algorithms as a resolution.



Al_2O_3 nanobowl compound, designed to isolate catalyst particles and improve fuel consumption processes. Data courtesy of Bin Liu, Maria Chan, Jeff Greeley (PI), ANL Center for Nanoscale Materials, and Larry Curtiss (PI), ANL Materials Science Division.

Materials Science

Using Quantum Chemistry to Study Photocathodes

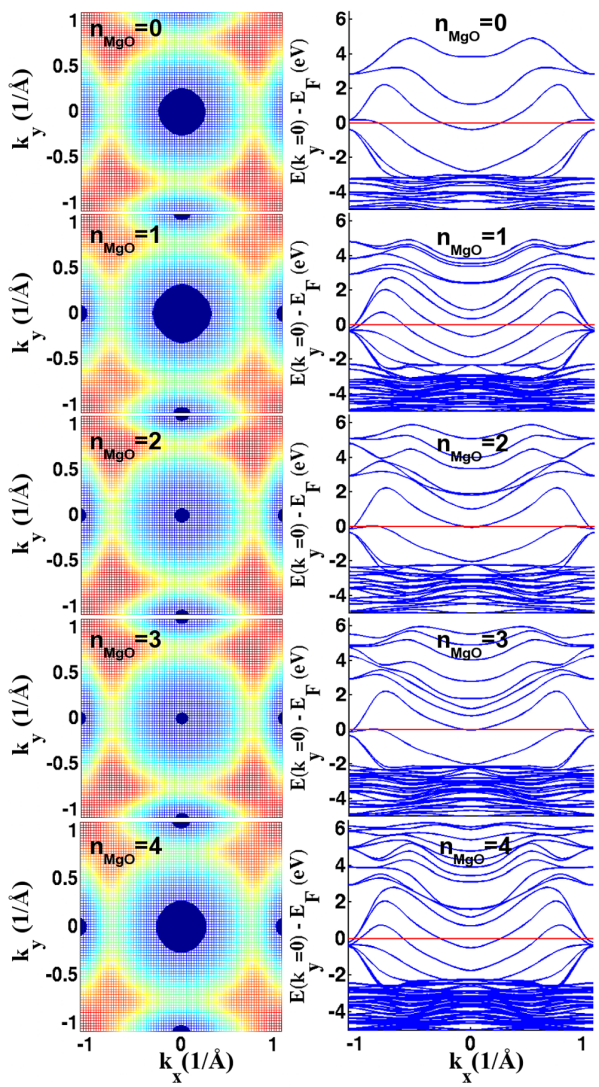
Preliminary Investigator: Karoly Nemeth, Argonne National Laboratory
Director's Discretionary Allocation: 0.5 Million Hours

Ultra-thin MgO films on Ag(001) surfaces constitute an example of how ultra-thin surface layers on metals can be used to control the emittance properties of photocathodes. In addition to substantially reducing the work function of the metal surface, the MgO layers also favorably influence the shape of the surface bands, resulting in the generation of high-brightness electron-beams. As the number of MgO surface layers varies from 0 to 3, the emitted electron beam becomes gradually brighter, reducing its transverse emittance to 0.06 mm-mrad.

Collaborators from Argonne, Northern Illinois University, and the Illinois Institute of Technology are developing photocathodes with ultra-low transverse emittance — a prerequisite for the development of x-ray free-electron lasers and energy-recovery linac x-ray sources. These devices can be employed to obtain sharper images of single, large molecules, such as vital proteins in physiological solutions. The research will contribute to the creation of instruments that will enable the study of phenomena that are not experimentally accessible today, including those in the biological and environmental research sector.

The research team is using the Quantum Espresso/PWSCF software package — a general quantum-mechanics code for atomic/molecular/solid-state physics and chemistry — to carry out the calculations of this work. The researchers are running their calculations on the Blue Gene/P at the Argonne Leadership Computing Facility and the Cray XT4 and XT5 at the National Energy Research Scientific Computing Center.

Researchers plan to conduct the screening of several other metal/oxide systems with the potential for low-transverse emittance photo-electrons by similar means. In addition, the team will study the effect of external electric field, surface roughness, etc. The best photocathode candidates will be tested experimentally.



Surface bands (left-hand panels) and the band structure (right-hand panels) of MgO(n_{MgO}ML)/Ag(001)(4ML)/MgO(n_{MgO}ML) systems in the Brillouin zone for n_{MgO}=0–4. Dark blue spots denote k-space regions with occupied electrons; otherwise, coloring indicates band height above E_F, the Fermi energy. Only surface bands with the highest energy occupied crystal orbitals in the center of the Brillouin zone are shown for each value of n_{MgO}.
Figure reproduced with permission from K. Nemeth et. al, Phys. Rev. Lett. *104, 046801 (2010).*

Nuclear Physics

Advancing the Understanding of Nuclear Structure

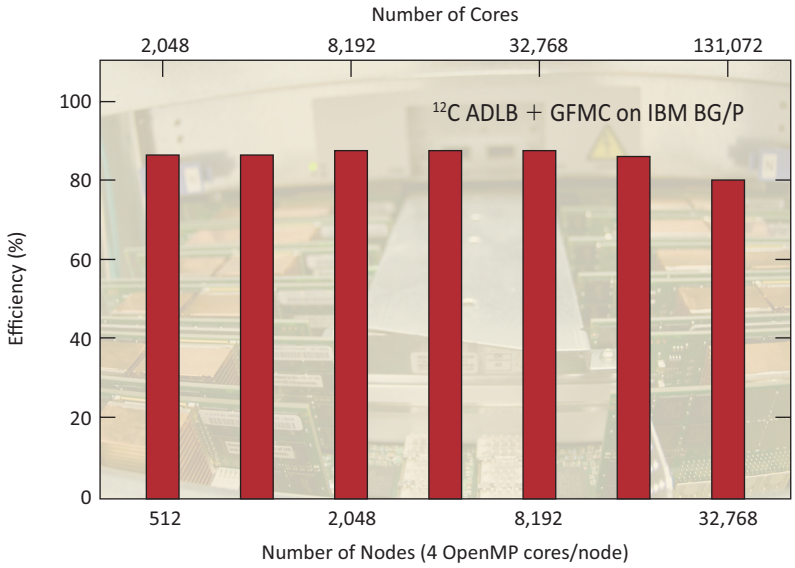
Principal Investigator: David Dean, Oak Ridge National Laboratory
INCITE Allocation: 15 Million Hours

Researchers from Oak Ridge and Argonne national laboratories are using complementary techniques, including Green's Function Monte Carlo, the No Core Shell Model, and Coupled-Cluster methods to perform *ab initio* calculations of both structural and reaction properties of light- and medium-mass nuclei. The calculations use realistic models of nuclear interactions including both two- and three-nucleon forces. Their work could advance understanding of the triple-alpha burning reaction, which is essential to life on earth.

They also are exploring the role of the three-nucleon force in substantially heavier nuclei. Furthermore, researchers are using Density Functional Theory (DFT) to calculate properties of nuclei across the entire range of nuclear masses. These DFT studies will help predict nuclear properties relevant to nuclear reactions such as neutron-nucleus reaction cross-sections and fission. This new understanding of nuclei has far-reaching implications, impacting the fields of energy and astrophysics. The researchers are conducting their calculations on the IBM Blue Gene/P (BG/P) at the Argonne Leadership Computing Facility and the Cray XT at Oak Ridge National Laboratory.

The BG/P research team has completed ground-state ^{12}C calculations — a key milestone. The ground state represents the best converged *ab initio* calculations of ^{12}C ever. The researchers have continued developing and testing various formulations of starting wave functions for the first excited 0^+ state of ^{12}C (the Hoyle or triple-alpha burning state). While they have not yet found a starting wave function that remains orthogonal to the ground state wave function during Green's Function Monte Carlo (GFMC) propagation, this work is ongoing.

The BG/P team has used the ^{12}C GFMC calculations to develop the Automatic Dynamic Load Balancing (ADLB) library, a general-purpose work-sharing library. By using OpenMP on each node, the team is now getting essentially perfect scaling up to 65,536 nodes (32,768 are used for their production runs). The team is now using the ^{12}C GFMC calculations to test a new version of ADLB that uses the MPI one-sided puts and gets.



Excellent scaling is achieved by the production Automatic Dynamic Load Balancing (ADLB) library on the BG/P.

Physics

Direct Multiobjective Optimization of Storage Ring Lattices for the APS Upgrade and Beyond

Principal Investigator: Michael Borland, Argonne National Laboratory
ALCC Allocation: 36 Million Hours

The brightest gets brighter

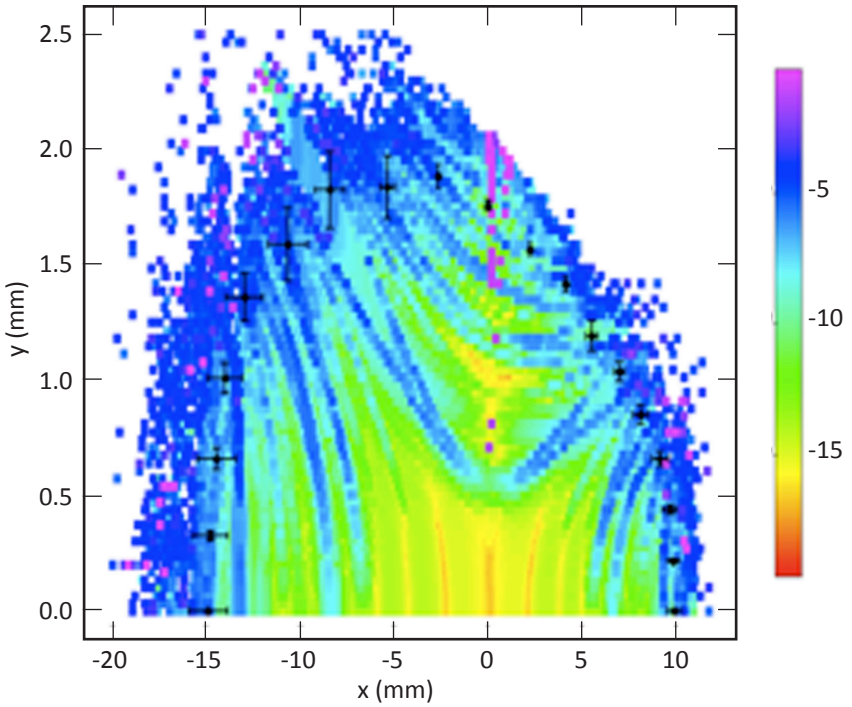
The brightest storage ring-generated x-ray beams in the Western Hemisphere are created by Argonne's Advanced Photon Source (APS) and are used by more than 5,000 scientists worldwide. A planned upgrade to the APS will reconfigure the facility's magnets (its "lattice") to enhance this world-class resource. The addition of long superconducting devices will increase brightness by an order of magnitude for x-rays above 20 keV. The upgrade will also accommodate systems for dramatically reducing the x-ray pulse length, giving the APS a unique position for enabling time-resolved science with hard x-rays. Without disruption to current operating modes, the upgrade will result in an improved source of high-energy, high-brightness, tunable x-rays for scientific research.

When massive compute power is elegant

Scientists at work on the APS upgrade are challenged with optimizing the nonlinear dynamics to provide both sufficient dynamic aperture (to ensure high-injection efficiency) and momentum aperture (to ensure sufficient beam lifetime). To tackle this challenge, researchers will pair the extreme computing power of the ALCF's Blue Gene/P with the APS-developed code "elegant" to create complex particle-tracking simulations.

Providing faster solutions today, building resources for tomorrow

The vast compute power of the Blue Gene/P gives scientists at work on the APS upgrade the ability to resolve more challenging problems faster. To keep pace with the community's seemingly insatiable appetite for increased brightness, researchers will use a portion of their ALCC allocation to advance important concept work for next-generation "ultimate" storage rings.



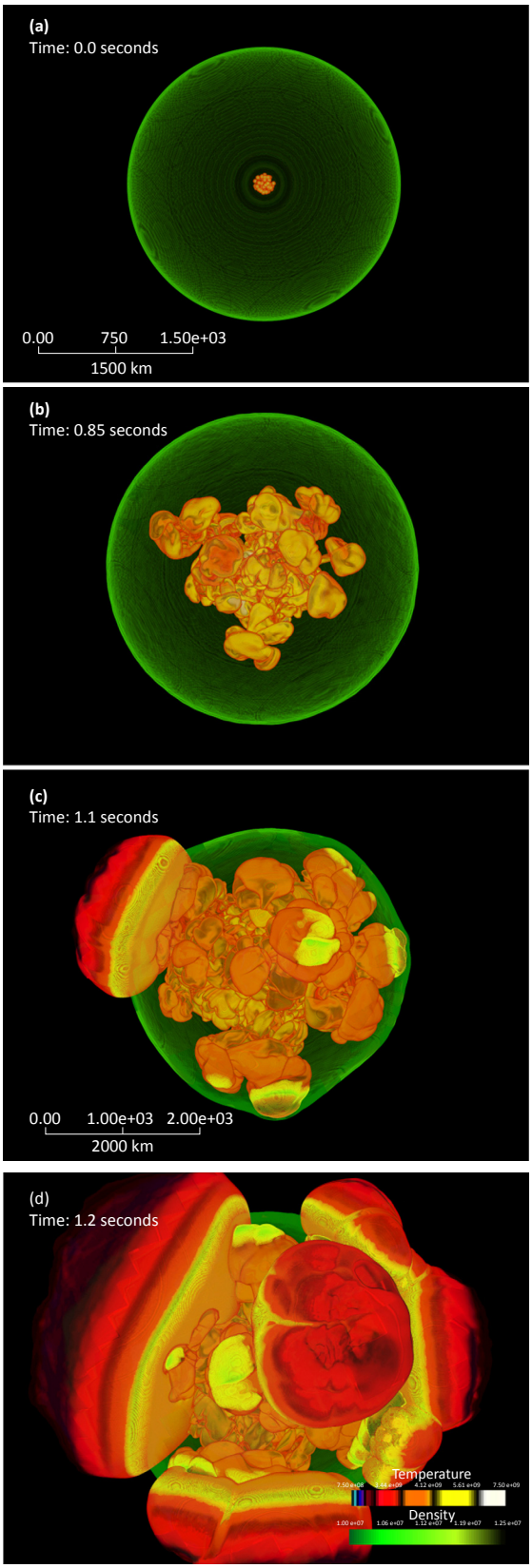
Dynamic aperture for 50 error ensembles overlaid on frequency map for APS-U lattice with SPX and Reduced Horizontal Beamsize insertions. The optimization process successfully excludes strong resonances from the interior region.

Physics

How Do Standard Candles Illuminate Knowledge of the Universe?

Principal Investigator: Donald Lamb, The University of Chicago

INCITE Allocation: 70 Million Hours



Type Ia supernovae (SNe Ia) are among the brightest exploding stars in the universe. Observations using SNe Ia as "standard candles" led to the discovery of dark energy. Most scientists believe that using SNe Ia to determine the properties of dark energy will require a much better understanding of these explosions.

Researchers are using the FLASH code and time on the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) awarded through the U.S. Department of Energy's INCITE program to conduct the first comprehensive, systematic validation of current models of SNe Ia and to determine the fundamental properties of buoyancy-driven turbulent nuclear combustion — a physical process that is key to SNe Ia but is not fully understood.

The team has simulated all current models of Type Ia supernovae on the ALCF's Blue Gene/P. These simulations led to the discovery of robust signatures for the different SNe Ia models, holding out the promise that observations can discriminate among them. The team also has simulated buoyancy-driven turbulent nuclear combustion. These simulations show 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.

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) × 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.

Physics

Nucleon Structure Down to the Physical Pion Mass

Principal Investigator: John Negele, MIT Center for Theoretical Physics
ALCC Allocation: 37.8 Million Hours

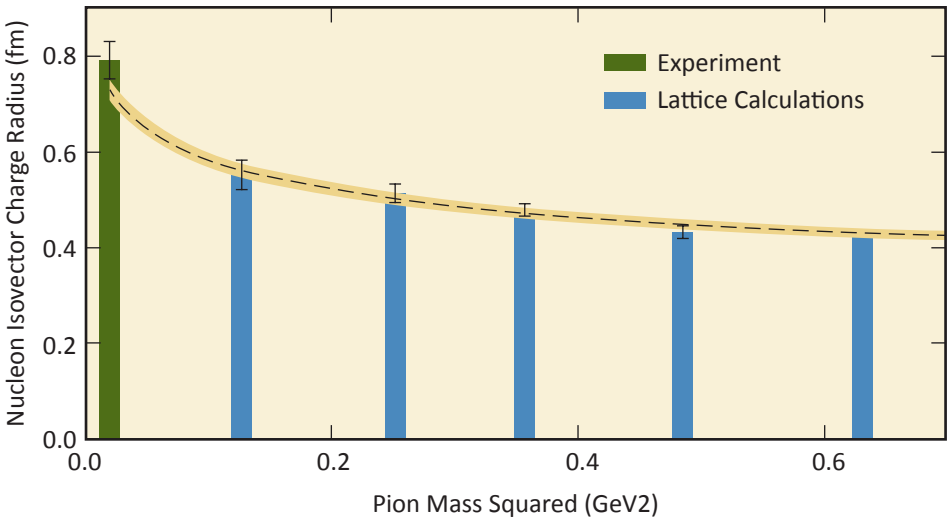
First-ever calculation of nucleon structure using full lattice QCD at the physical pion mass

Researchers led by John Negele from MIT's Center for Theoretical Physics will use their ALCC allocation to perform the first calculation of nucleon structure using full lattice QCD at the physical pion mass. Working with the Budapest-Marseille-Wuppertal (BMW) collaboration and using their 2+1 flavor dynamical stout-smeared O(a)-improved Wilson quark configurations for nucleon structure observables, they will calculate connected diagram contributions to form factors, moments of structure functions, and generalized form factors at 6 pion masses from approximately 338 MeV down to the physical pion mass at lattice spacing ~ 0.12 fm.

The team will study scaling behavior by calculating observables for m ~ 250 MeV at a ~ 0.12, 0.09, and 0.07 fm and finite volume corrections effects by comparing results for mL = 4.1 and 5.5 at m = 296 MeV. They will also conduct an extensive calculation of disconnected quark diagrams and gluon contributions for m ~ 250 MeV at a ~ 0.12 fm.

Optimized code, exceptional performance

The software for the stout-smeared O(a)-improved Wilson fermion calculations was optimized by Stefan Krieg for the Blue Gene/P. At these lattice sizes, the Dirac operator achieves a maximum of 37 percent of peak and typically runs at approximately 32 percent of peak on one to sixteen racks. The full inverter runs at more than 32 percent of peak. Using their own optimized domain wall inverter, performance is exceptional and provides significant advantage to the U.S. lattice QCD effort of international QCD software development supported by ASCR and NNSA.



Fundamental properties of the nucleon, such as the charge radius shown here, can be calculated from first principles by solving QCD numerically on a space-time lattice. This figure shows results featured in the DOE NSAC long-range plan, which had to be extrapolated from the left-most blue point to the physical pion mass shown in red. The goal of the current project is to calculate the radius at several masses lower than the lightest blue point as well as at the physical pion mass, to remove any extrapolation ambiguity.

Physics

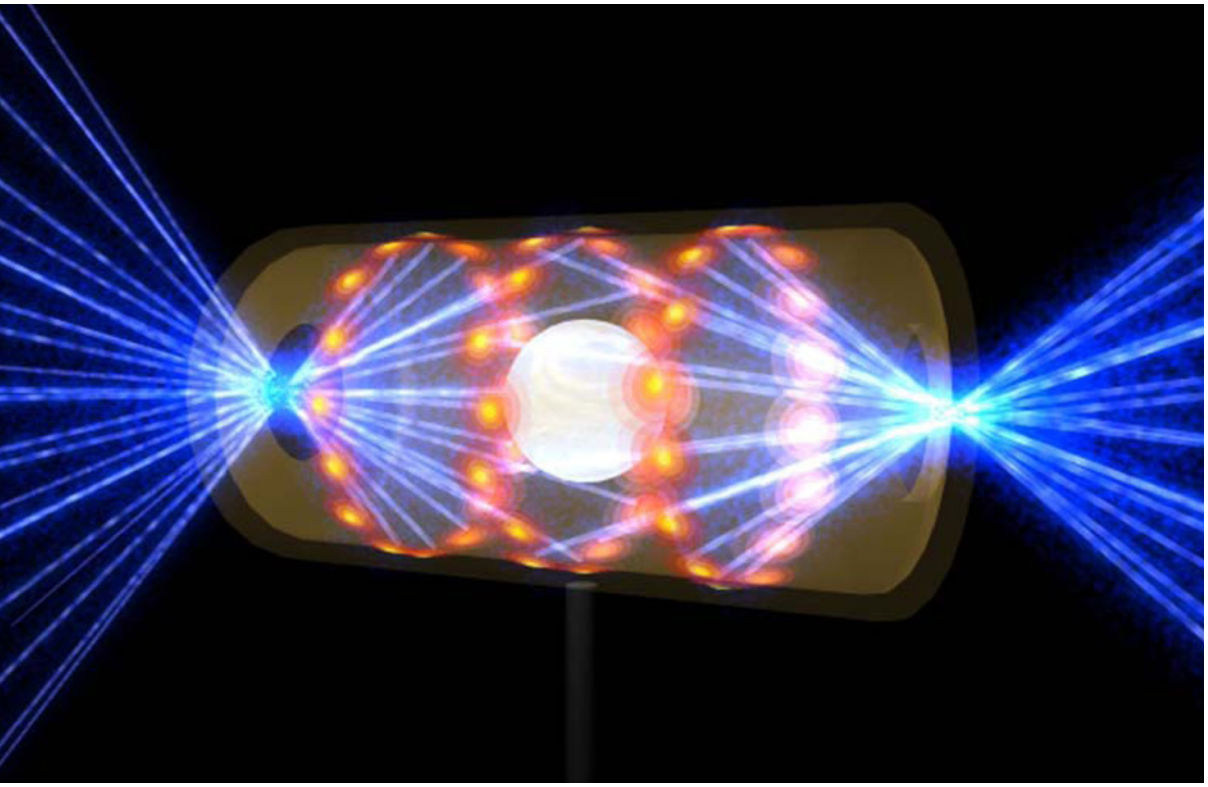
Simulating Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond

Principal Investigator: Denise Hinkel, Lawrence Livermore National Laboratory
INCITE Allocation: 45 Million Hours

Lawrence Livermore National Laboratory (LLNL) has been tasked with achieving ignition at the National Ignition Facility (NIF). An important aspect of the ignition campaign involves quantitative prediction of the level of laser backscatter in these targets. Mitigation of laser backscatter is important, as backscatter reduces the amount of input energy available for driving the fusion process. It can also alter implosion symmetry as well as preheat the ignition capsule via generation of hot electrons.

Recent experimental results from the National Ignition Campaign at NIF show that backscatter occurs in the laser target where quads of laser beams are overlapped. The goal of these simulations is to quantify how overlapping beam quads impact laser backscatter. In the first simulation completed, which ran on the full BG/P Intrepid machine at Argonne, three quads of NIF beams propagated 750 micrometers, through half of the interaction region where laser backscatter occurs (113 billion zones). The beams were not polarization smoothed, a technique used at NIF to reduce laser backscatter. (Simulating the full backscatter region or including polarization smoothing results in a simulation too large for the full Intrepid machine.) Laser backscatter primarily occurs in the left and right beam quads because the resonance region for the central beam quad is marginally included in this simulation.

The simulations being conducted by LLNL researchers will generate scientific results that will have a major impact on the national ignition campaign — inertial fusion — as well as on the fundamental science of LPI. These state-of-the-art simulations are only possible because of the INCITE award received on the Argonne BG/P Intrepid machine.



NIF Hohlraum. This artist's rendering shows a NIF target pellet inside a hohlraum capsule with laser beams entering through openings on either end. The beams compress and heat the target to the necessary conditions for nuclear fusion to occur. Ignition experiments on NIF will be the culmination of more than 30 years of inertial confinement fusion research and development, opening the door to exploration of previously inaccessible physical regimes. Credit: Lawrence Livermore National Laboratory.

OPERATIONS

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

Computing Resources

The Argonne Leadership Computing Facility systems are research machines open to Department of Energy INCITE projects and other select users.

Intrepid

The ALCF state-of-the-art system gives the computational science community a computing capability dedicated to advancing knowledge towards solving humanity's most challenging scientific problems.

Blue Gene/P has a highly scalable torus network that can accommodate configurations with a petaflop of peak performance, as well as a high-performance collective network that minimizes the bottleneck common in simulations on large, parallel computers. Intrepid uses less power per teraflop than systems built around commodity microprocessors, resulting in greater energy efficiency and reduced operating costs. Blue Gene applications use common languages and standards-based MPI communications tools, so a wide range of science and engineering applications are straightforward to port, including those used by the computational science community for cutting-edge research in chemistry, combustion, astrophysics, genetics, materials science and turbulence.

Eureka provides users with visualization and data analytics to transform data into useful knowledge.

Intrepid (Blue Gene/P) — the ALCF's production machine for open science research

- 40,960 quad-core compute nodes
- 163,840 processors
- 80 terabytes memory
- 557 teraflops

Surveyor

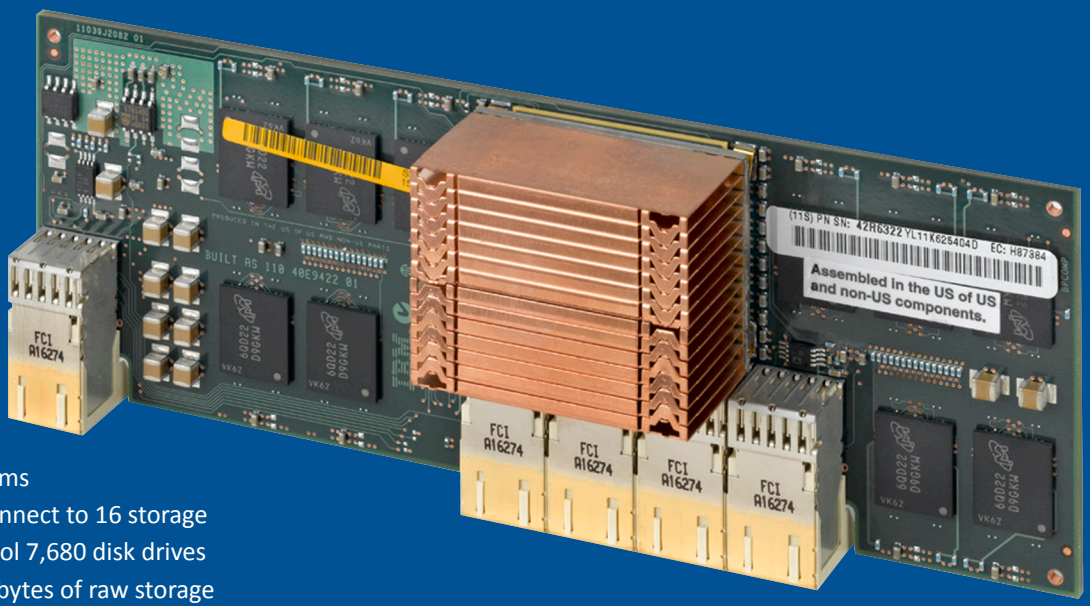
ALCF's Surveyor is a Blue Gene system dedicated to tool and application porting, software testing and optimization, and systems software development. Surveyor has 1,024 quad-core nodes (4,096 processors) and two terabytes of memory. Peak performance is 13.9 teraflops.

Eureka

Most science applications that run on large-scale systems like Intrepid at the Argonne Leadership Computing Facility (ALCF) generate huge volumes of data that represent science results. Researchers analyze and explore this data output, and often convert the data to visual representations. To facilitate data analytics and visualization at the ALCF, researchers employ Eureka, one of the world's largest installations of NVIDIA Quadro Plex S4 external graphics processing units (GPUs). By using the NVIDIA visual computing system as the base graphics building block, Eureka enables breakthrough levels of productivity and capability in visualization and data analysis.

Eureka — the ALCF's visualization and data analytics solution

- 100 dual quad-core servers
- 200 Quadro FX5600 GPUs
- 111 teraflops
- more than 3.2 TB of RAM



Gadzooks

Gadzooks is the ALCF's test and development system for visualization. It has four compute nodes, each with two 2.0 GHz quad-core Xeon servers with 32 GB RAM and eight NVIDIA Quadro FX5600 GPUs in two S4s.

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 access the storage. The tape drives have built-in hardware compression allowing compression ratios of between 1.25:1 and 2:1, depending on the data, giving an effective capacity of 16–24 petabytes. An HPSS automated tape storage system provides archival storage with 16,000 tapes in two 10,000-slot libraries.

Networking

The Blue Gene/P uses five different networks for different communication operations. The 3D 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 3D torus network is also usable as a 3D mesh. The supercomputer connects to other research institutions using a total of 30 Gb/s of public network connectivity. Scientists can 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).

Cloud Computing

Magellan, a new cloud project funded by the American Recovery and Reinvestment Act through the U.S. Department of Energy (DOE) is examining cloud computing as a potential new computing paradigm for scientists to accelerate discoveries in a variety of disciplines. 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 installed different storage hardware and environments. The combined set of systems created a cloud testbed that scientists can use for their computations while also testing the effectiveness of cloud computing for their particular research problems. The ALCF and NERSC facilities are 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.

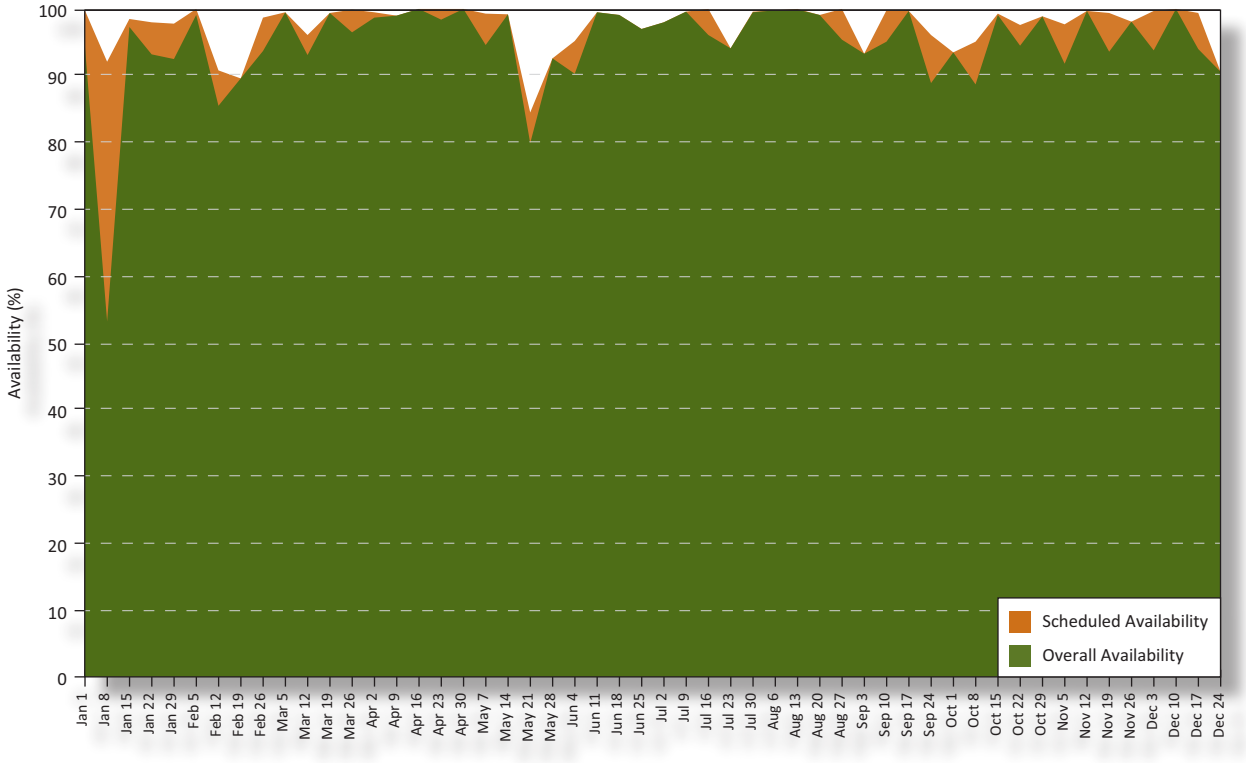
Intrepid Offers High Availability, Utilization

The ALCF (and most data centers) track availability, also known as uptime, and consider it one of their key metrics. ALCF Operations tracks two types of availability: scheduled and overall. Scheduled availability is simply what percentage of the time the ALCF said the machine would be available, and was it really available? Overall availability is what percentage of the time the machine could theoretically have been available, and was it available? The former is sensitive to unscheduled failures, while the latter is sensitive to unscheduled failures, as well as scheduled downtime (maintenance). As an example, if staff scheduled four hours of maintenance on a particular day, but due to unanticipated problems, it took eight hours, then the scheduled availability would be (24–8)/(24–4) = 80%. The ALCF said it would be available for 20 hours on that day, but it was only available for 16. The overall availability would be 24–8/24 = 66.6%. The machine could have been available for 24 hours in this example, but it was only available 16.

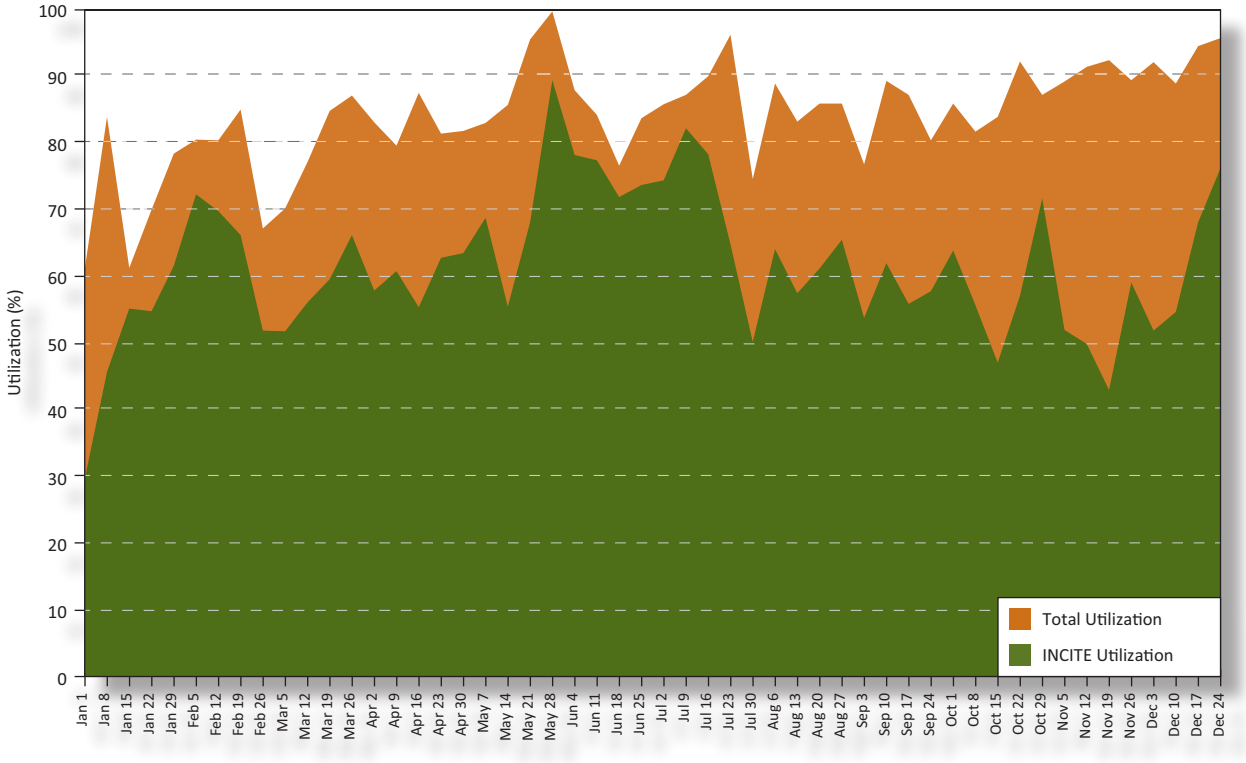
The ALCF is required to deliver a minimum of 95% scheduled availability and 90% overall availability. ALCF staff worked with DOE to analyze the tradeoffs between the cost of downtime, the cost of the infrastructure, and the probability of lost time and concluded that this was the most cost-effective design point. Note that in the example, staff used simple wall clock time to keep the math simple. However, in reality, the machine can be partially down (a node, or a single rack might be down, but the rest are running), so the staff actually tracks it in terms of core hours (i.e., the same type of accounting is used for each core in the machine).

The ALCF also tracks utilization. Conceptually, utilization is simple. Of the hours the machine was available, how many hours was it being used, and how many hours was it sitting idle? Unfortunately, that is where the simplicity ends. Utilization is a complex balance between competing factors, particularly for the leadership facilities, where running large jobs is one of our primary goals. As an example, if every job were a single node, then getting high utilization would be easy. Any time a job ended, as long as there was a job in the queue ready to go, it would “fit” on the resource that was available.

The same would be true at the other extreme: If all jobs were 40 racks (the same size as the whole machine), the scheduling would be easy. What the ALCF actually receives are jobs of varying sizes and durations and a very complex “game of tetris” trying to make all the pieces fit. Staff also has to balance user wait times, etc. Bigger jobs require a higher priority, but everyone has to get their work done in a reasonable amount of time. The utilization on Intrepid runs in the 80% - 85% range, which is considered good for leadership facilities.



Availability, averaged by week, for the period January 1, 2010 to December 31, 2010.
Orange "spikes" represent significant planned downtime. (There was a Myricom network upgrade in January.)
White "valleys" represent significant unplanned downtime. (There was a chiller failure in May.)



Utilization by allocation category, averaged by week, for the period January 1, 2010 to December 31, 2010.

STAFF & SERVICES

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

Catalysts

The Catalyst Team provides key projects with an assigned expert to maximize and accelerate their research.

Features include:

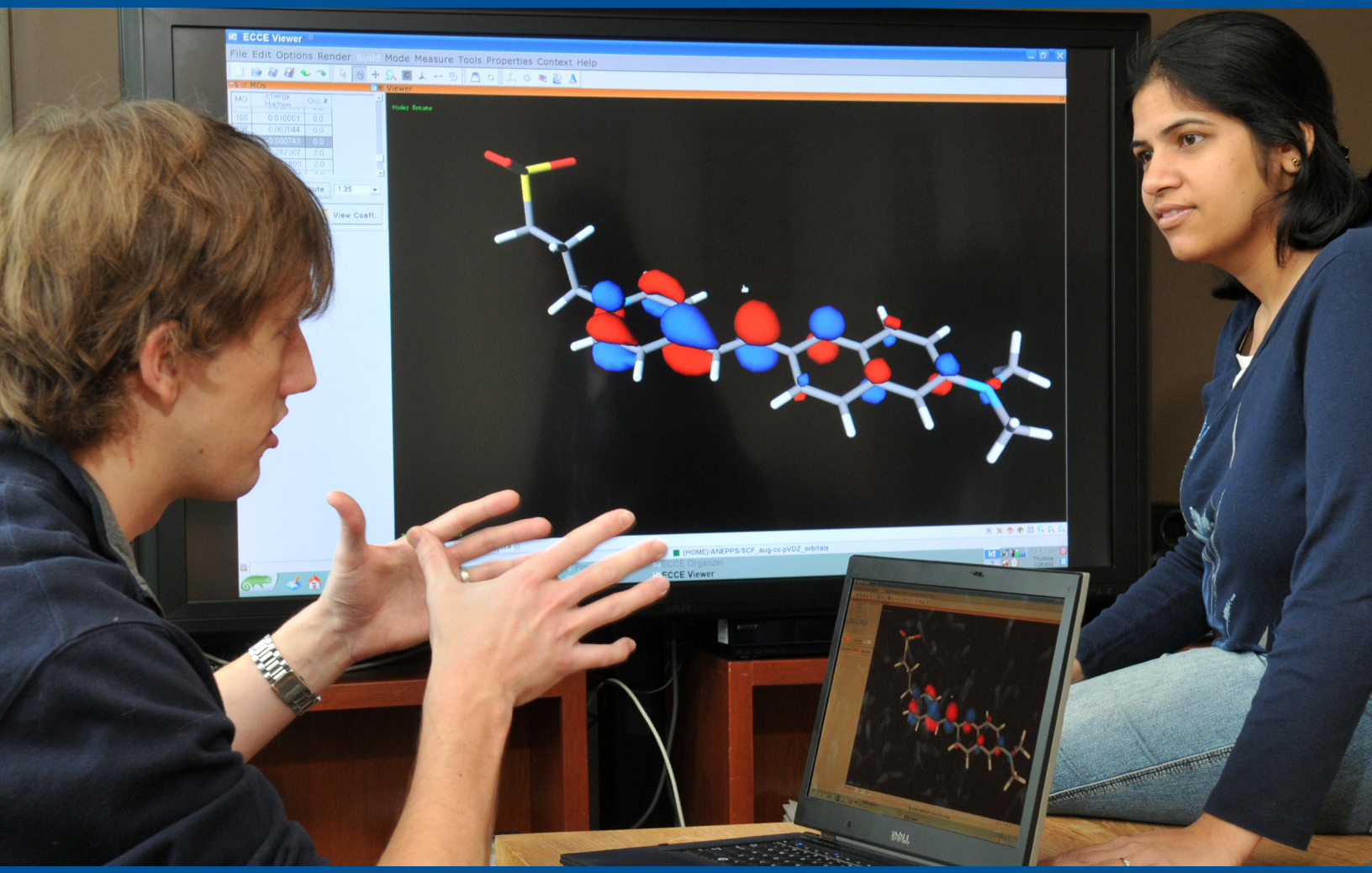
- Full project lifecycle assistance
- Catalysts are experienced computational scientists in domains that reflect the user community as well as possessing in-depth knowledge of computational approaches that are effective on ALCF systems
- Tailored services for unique requirements of a given research initiative
- Access to assistance and coordination from an assigned ALCF catalyst

The Catalyst Team:

- Provides a "jump-start" in the use of ALCF resources
- Aligns the availability of ALCF resources with the needs of the project team
- Establishes a spirit of collaboration to maximize the value that ALCF can bring to our project partners

"This year, the entire team dug deep and spent a lot of time on the INCITE program, new ALCC and ESP programs, and Blue Gene/Q preparation. We welcomed several new Catalysts and had a wildly successful year with the science conducted at the ALCF."

Katherine Riley
Group Leader



Key Accomplishments

- Early Science Program
  - Successfully started the Early Science Program (ESP) in 2010.
  - Issued an open call for ESP proposals and conducted a full review and selection process for all proposals.
  - Held a large ESP kickoff workshop on October 18–19, 2010.
  - Started an aggressive recruiting effort for 15 post-docs.
- INCITE Proposal Review
  - Reviewed 125 INCITE proposals within two months; ultimately, 30 ALCF projects — 18 new and 12 renewals — were selected for 2011.
- SC10 Activities
  - Group Leader Katherine Riley served as SC10 Tutorials Committee Co-Chair.
  - Team members presented SC10 posters, papers, and presentations.
- Catalyst Team Publications:
  - Catalysts co-authored ~15 papers and presentations in 2010.

Data Analytics and Visualization

The Data Analytics and Visualization team has expertise in tools and methods for high-performance post processing of large datasets, interactive data exploration, batch visualization, and production visualization.

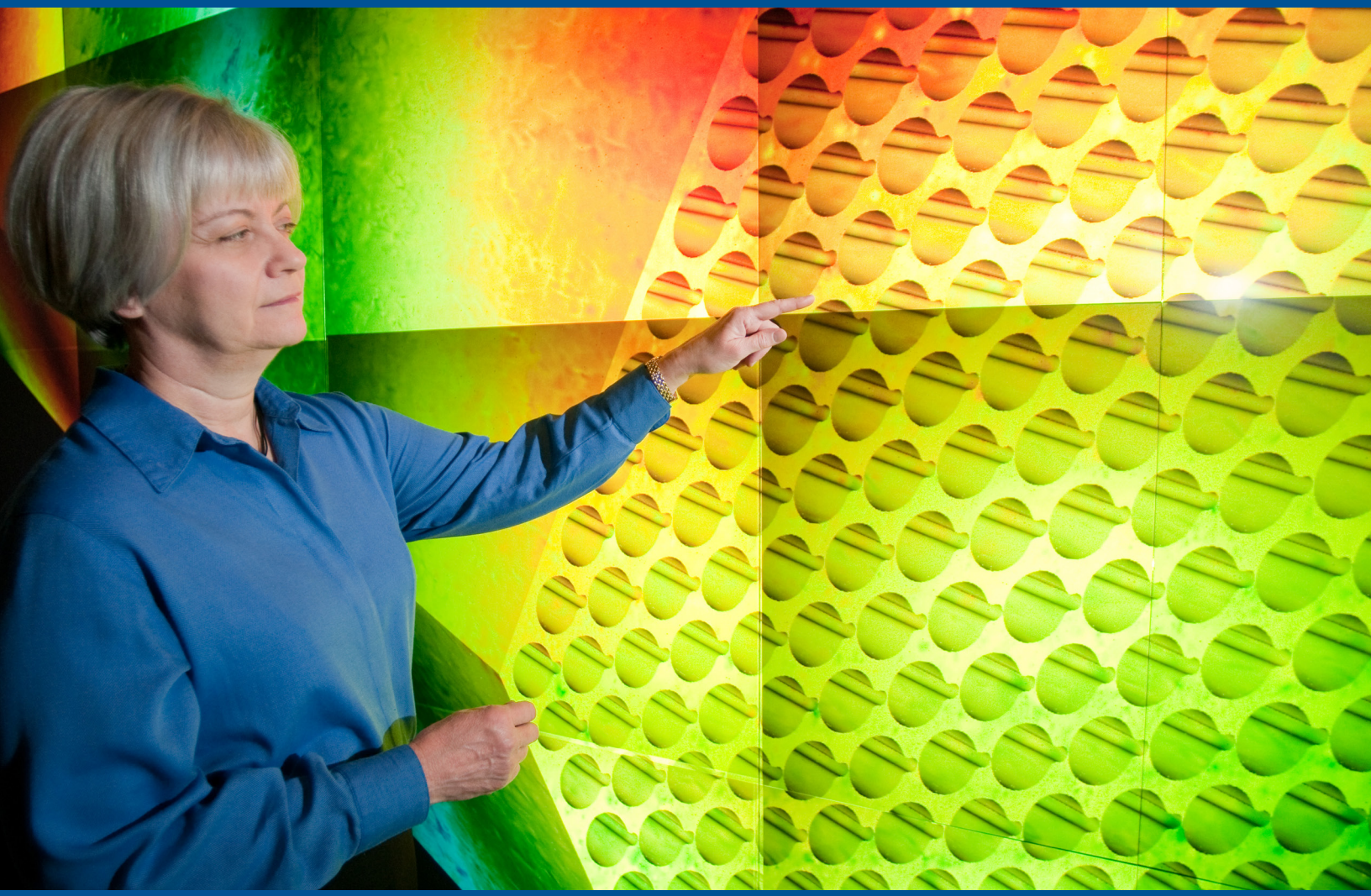
We help users with their visualization and analysis needs using ALCF high performance resources and a suite of tools maintained for these purposes. To this end, we provide help in these key areas:

- Production tools for high-performance visualization (ParaView, VisIt)
- Analysis tools (R, MATLAB)
- Presentation graphics (PowerPoint, Keynote, Final Cut Pro)

The ALCF Data Analytics and Visualization team has strong connections to MCS R&D in the area of visualization and analysis.

"We have been able to engage more users this year than in any previous year, leading to groundbreaking visualizations, new collaborations, and a better informed cadre of users."

Mark Hereld
Group Leader



Key Accomplishments

- The Data Analytics and Visualization (DA&V) team worked with Brown University researchers to develop new multi-part visualizations of blood flow simulations. Visualization results from this work were presented at SC10.
- Researchers at GE Global Research and the DA&V team developed new visualizations of complex turbulent mixing noise sources in jet exhaust nozzles. Visualization results from this work were presented at SC10 and featured on the cover of the recent ASAC 2010 Fall Report.
- Eureka produced animations of FLASH simulations of Type Ia supernovae as cosmological standard candles, the basis for measuring the expansion of the Universe and experimental understanding of dark energy.
- Studies of galaxy cluster mergers using FLASH were visualized using Eureka.
- HEDP simulations of laser-driven instabilities on a material sample resulted in detailed movies rendered on Eureka.
- Detailed simulations of sodium-cooled fast reactor (SFR) coolant flow in a model of a reactor fuel bundle were visualized on Eureka.
- Visualizations using a variety of tools helped scientists study nano-structures — from interactions between gold atoms and nano-particles of sapphire to the evolution and dynamics of nano-bowls.
- The team led workshops to teach users how to apply facility visualization and analysis tools and platforms to their science.
- Working with computer scientists from Argonne's Mathematics and Computer Science Division, the team published a paper at SC10 on new methods for improving performance of data movement in supercomputing platforms such as Intrepid.

Operations

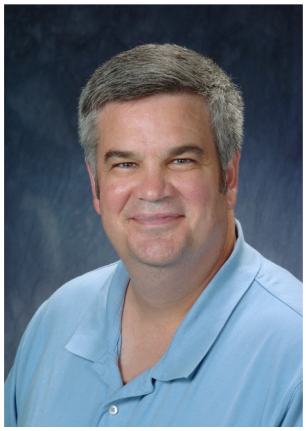
The ALCF Operations team consists of the Systems Group and the Advanced Integration Group.

The Systems Group is responsible for:

- Hardware maintenance
- Software maintenance
- Resolution of user tickets related to system issues
- Responding to requests for new software or versions of software
- Developing systems tools, particularly ones related to the unique system architectures and scale of ALCF resources.

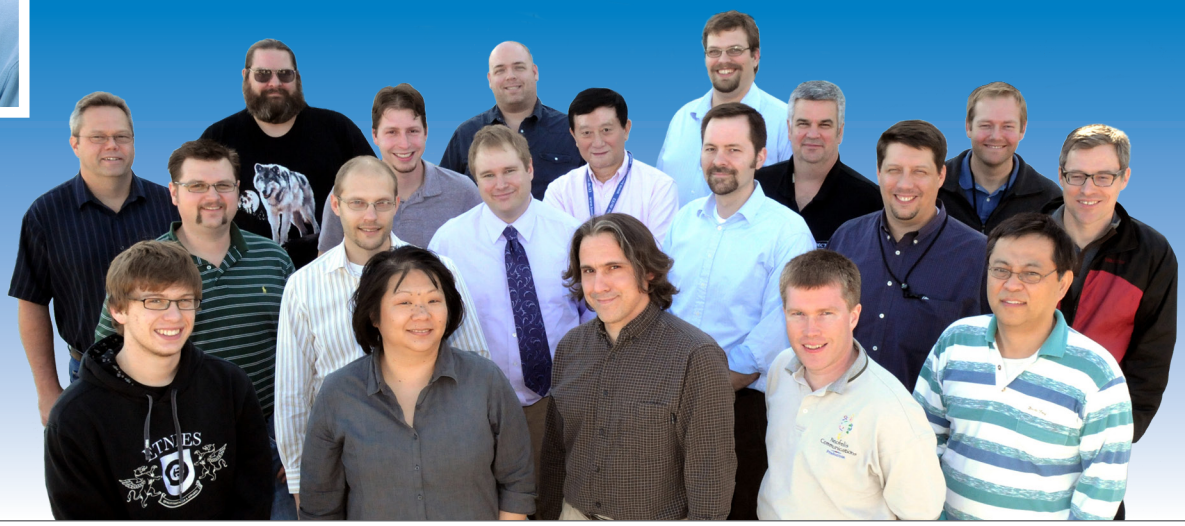
The Advanced Integration Group is responsible for:

- Ensuring the entire system software stack works together
- Assisting with I/O performance issues
- Addressing bug fixes and feature requests for systems software, which includes, but is not limited to:
  - Responding to requests for new software or versions of software
  - The clusterbank job accounting system
  - The PVFS file system
  - The Darshan I/O monitoring library
  - Internal and external report generation
  - Exploring new hardware and software
  - The Cobalt job scheduling system technologies for our next generation systems



Bill Allcock
Group Leader

"Due to the fantastic skills and efforts of the Operations team, we've dramatically improved the stability of the Blue Gene/P system and will continue to make further enhancements in the future."



Key Accomplishments

- The team installed a dedicated filer that reduced boot failures due to network file system timeouts to zero, decreased boot times by up to 50%, and provided other internal operational benefits.
- Reporting is faster, more efficient and accurate due to the real-time database capture of system reliability, availability, and serviceability events and Cobalt scheduler logs.
- All known serious hardware issues on the machine have been eliminated to date.
- The system's availability metric has been significantly exceeded.
- Jointly working with Argonne's Facilities Management and Services personnel, the team improved the stability of the chiller infrastructure, leading to reduced downtime.
- The team brought Magellan, a cloud computing research infrastructure, online.
- Planning was initiated for a major storage upgrade in 2011.

Performance Engineering

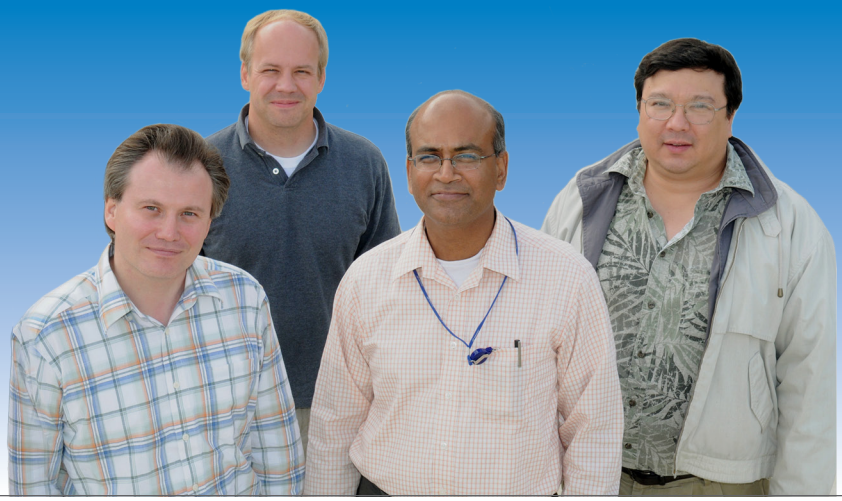
The mission of the Performance Engineering group is to ensure the effective use of applications on the Blue Gene/P system by assessing and improving the algorithms used by applications and the techniques used to implement those algorithms. This team's efforts are driven by the needs of the applications.

ALCF Performance Engineers have extensive expertise in:

- Application scaling and single core optimizations
- Performance modeling and projections
- Performance tools and libraries
- Benchmark development
- Computer architectures

"We are pleased that Intrepid ranked #1 on the Graph 500, demonstrating its balanced architecture to support data-intensive supercomputing applications."

Kalyan Kumaran
Group Leader



Key Accomplishments

- The ALCF's Intrepid ranked #1 on the first Graph 500 list unveiled at SC10 in November. The list ranks supercomputers based on their performance on data-intensive applications and thus complements the Top 500 list that is based on the LINPACK benchmark.
- Improved performance and scaling of several key INCITE and ALCC applications, including NWChem, HIRAM, GFMC, FLASH, GTC, Nektar, Frontier, etc.
- Took part in the Extreme Scaling Workshop, held March 22–24, 2010, at the Juelich supercomputing centre, and successfully ran the largest-ever NEK5000 simulation on more than 290 K cores of Juegene.
- Coordinated an ALCF next-generation Blue Gene performance project for porting community tools and libraries and programming models. Lead the project.
- Led three ALCF workshops and external presentations at ScicomP and CScADS workshops.
- Participated actively in SPEC HPG and OpenMP ARB standard consortiums and in IBM SP-XXL and ScicomP user groups.

User Services and Outreach

The USO team provides frontline services and support to existing and potential ALCF users. The team also provides marketing and outreach to users, DOE and the broader community.

The USO provides the following services:

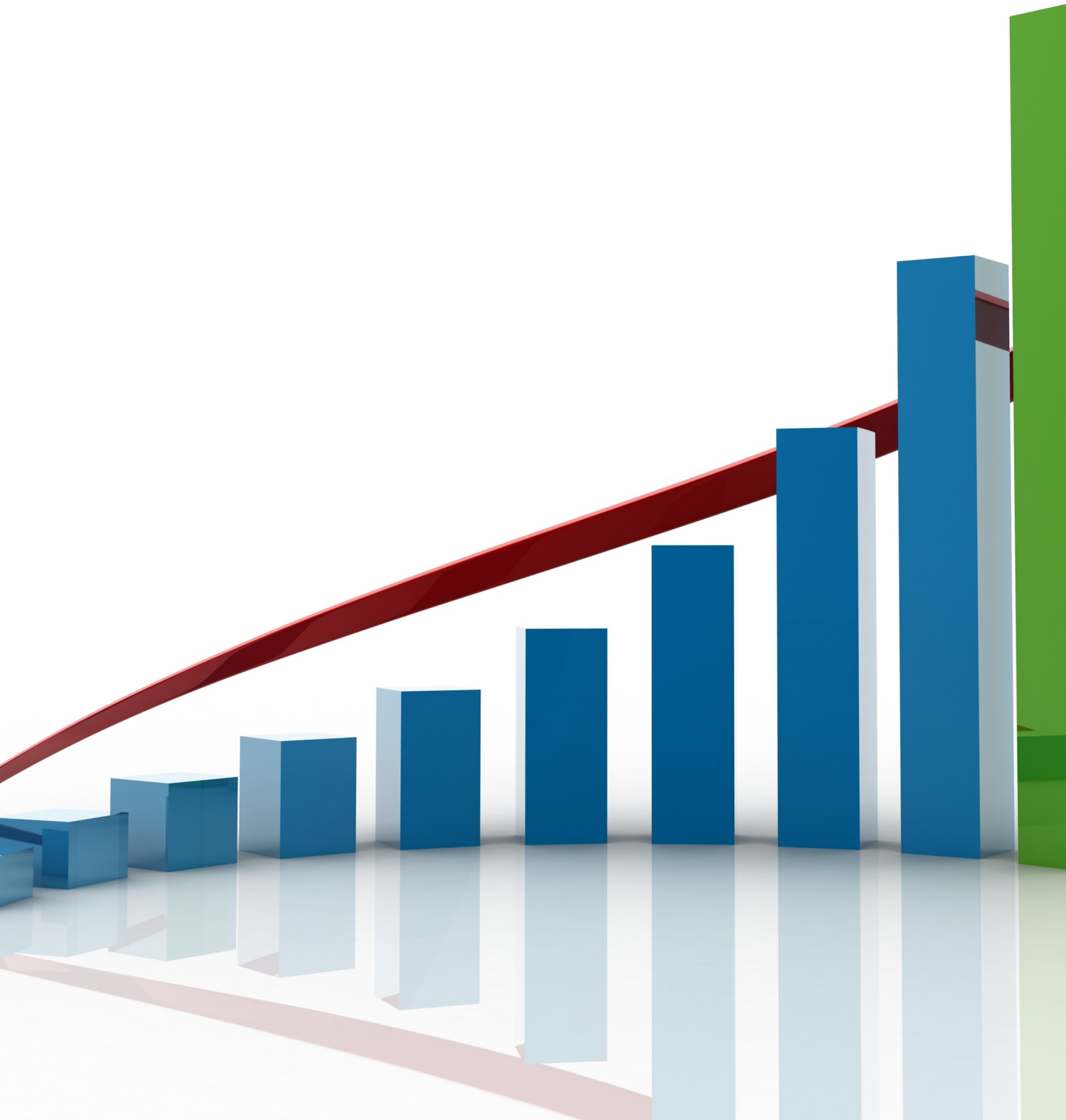
- Account/Project Administration
  - Account creation and administration
  - Project creation and allocation managements
  - User access and foreign clearance processing
  - Setup of crytocard and ssh access
- Training and Education
  - Monthly INCITE/ALCC user call
  - Workshops and conferences
  - Website technical content
- Help Desk
  - Immediate answers to questions
  - Triage and troubleshoot problems
  - Escalation to appropriate resource
- User Outreach
  - Website content
  - Index of user publications
  - Facility tours
  - Public relations and media coordination
  - Displays, education materials

David Martin
Group Leader

"Thanks to the dedication of the user services and outreach staff, ALCF dramatically increased the number of projects and users supported, while simultaneously increasing user satisfaction."

Key Accomplishments

- The ALCF user base is a highly sophisticated group, and the ALCF strives to work in collaboration with each user. The number of users supported by the ALCF continued to rise in 2010.
- The ALCF service desk responds to a wide variety of issues, from a simple password reset to complex hardware errors. The ALCF receives an average of 1,546 new tickets per month from users. During 2010, 79% of user tickets were addressed by the User Services and Outreach (USO) team within three working days.
- More than 90% of ALCF users rated their experience with the ALCF in 2010 as excellent or above average.
- More than 200 attendees participated in ALCF-sponsored workshops in 2010. New users were introduced to the ALCF at the Getting Started workshop, established users took their codes to the next level at the Leap to Petascale workshop, and potential users from around the globe logged into a webinar, where they learned tips and tricks for writing a successful INCITE proposal. In addition, the ALCF hosted an orientation workshop for the Early Science Program researchers — a group selected to be the first users on the ALCF's next-generation Blue Gene/Q system. And Deputy Division Director Susan Coghlan gave Argonne scientists their first look at the ARRA-funded cloud testbed, Magellan.
- ALCF staff actively participated in SC10 through papers, presentations, and a strong presence at the Argonne booth.



USER STATISTICS

SCIENCE POWERED BY SUPERCOMPUTING

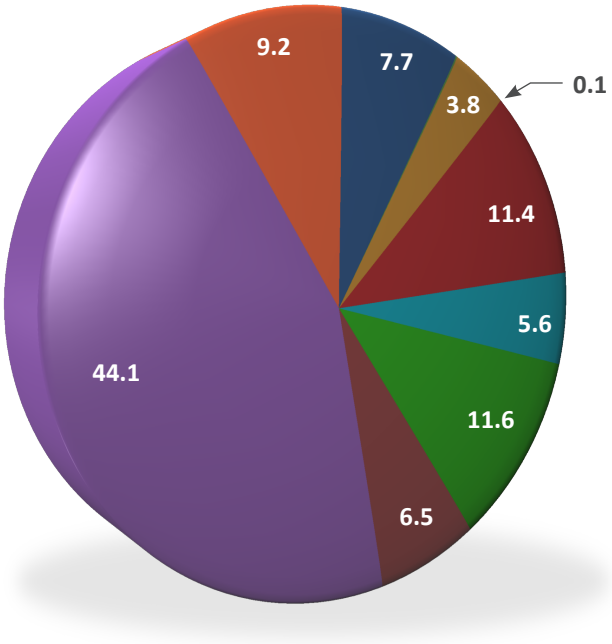
2010 ANNUAL REPORT

Producing More Science per Watt for a GREENER America

The Argonne Leadership Computing Facility meets the demands of the advanced simulation and modeling community while addressing important environmental concerns.

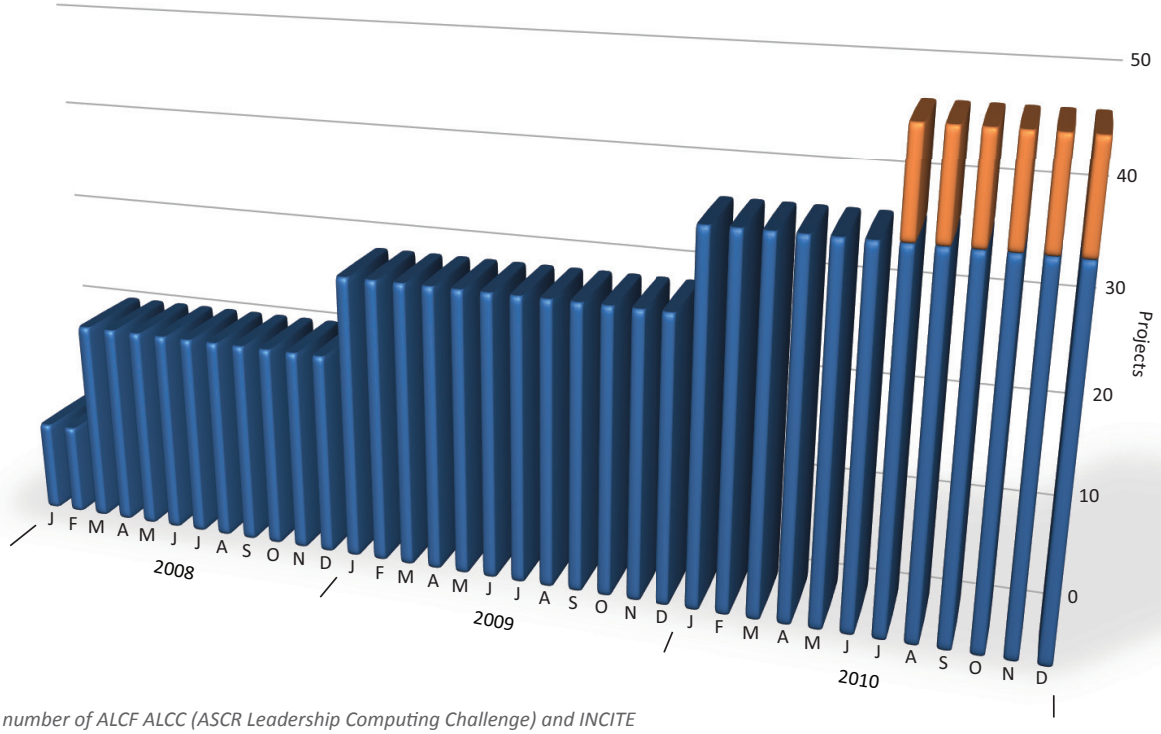
- Similar computing centers require several megawatts of electricity — enough to power a small town! The ALCF needs just over one megawatt of power.
- The energy efficiency of the ALCF saves taxpayers more than a million dollars a year.
- Our supercomputer, the Blue Gene/P, uses a third the electricity of comparable machines built with conventional parts.
- Cold Chicago weather chills the water used to cool the machine room for free several months of the year.

2010 INCITE, Discretionary, and ALCC Projects

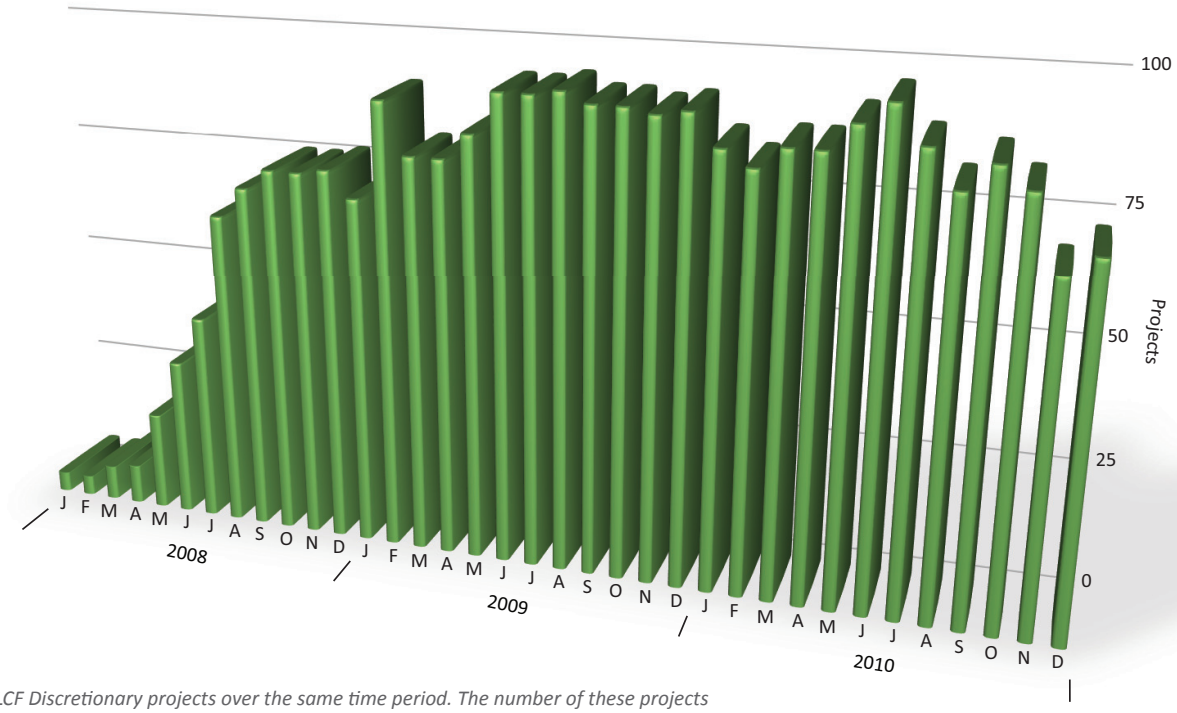


- Biological Sciences
- Workshops
- Computer Science
- Earth Science
- Materials Science
- Engineering
- Energy Technologies
- Physics
- Chemistry

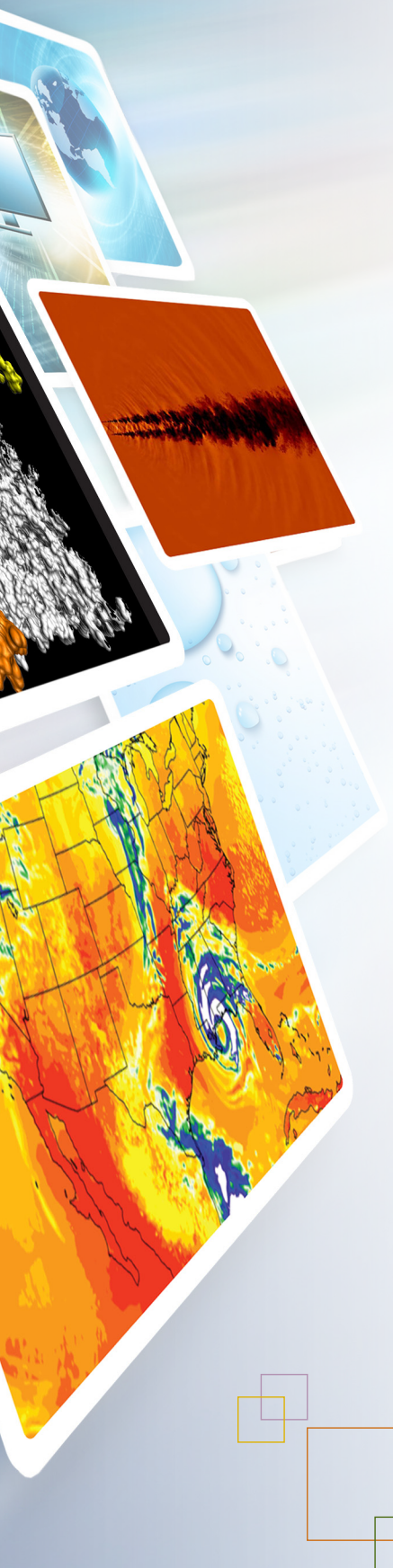
Percentage of hours used for each scientific discipline on the Blue Gene/P system from January 1, 2010–December 31, 2010.



The number of ALCF ALCC (ASCR Leadership Computing Challenge) and INCITE (Innovative and Novel Computational Impact on Theory and Experiment) projects since 2008.



ALCF Discretionary projects over the same time period. The number of these projects fluctuates over time, because Discretionary projects can begin at any time, and many are active for only a few months.



LOOKING AHEAD

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

Blue Gene/Q: The Next Generation

Argonne will use IBM's next-generation Blue Gene supercomputer to enable significant advances in areas such as designing ultra-efficient electric car batteries, understanding global climate change, and exploring the evolution of our universe.

The 10-petaflops IBM Blue Gene/Q supercomputer, named "Mira," will be delivered in 2012 and made available to scientists from industry, academia, and government research facilities around the world.

"Computation and supercomputing are critical to solving some of our greatest scientific challenges, like advancing clean energy and understanding the Earth's climate," said Rick Stevens, associate laboratory director for computing, environment, and life sciences at Argonne National Laboratory. "Argonne's new IBM supercomputer will help address the critical demand for complex modeling and simulation capabilities, which are essential to improving our economic prosperity and global competitiveness."

Argonne National Laboratory will use IBM's next-generation Blue Gene/Q supercomputer to stoke economic growth and improve U.S. competitiveness for such challenges as designing safer and more efficient combustion mechanisms, modeling cellular-scale biological processes to address human health issues, and studying nuclear physics reactions of critical importance to neutrino detector and accelerator experiments. The system will be four times as fast as today's fastest supercomputer, providing a strong science and technology engine that will fuel national innovation.

Mira will be 20 times faster than the ALCF's IBM Blue Gene/P, Intrepid, running programs at 10 quadrillion calculations a second. If every man, woman and child in the United States performed one calculation each second, it would take them almost a year to do as many calculations as Mira will do in one second.

The Argonne Leadership Computing Facility (ALCF) is already working with potential users as part of the "Early Science Program," a program designed to get researchers working on the most effective ways to leverage the computer's power as soon as it is deployed.

Argonne and DOE have selected 16 projects from a pool of proposals, in a wide variety of disciplines, which will be the first to gain access to Mira's capabilities. These span a diverse range of projects from reducing energy inefficiencies in transportation and developing advanced engine designs to spurring advances in energy technologies. The progress made during the Early Science Program should enable researchers to quickly leverage Mira's computational capability to reach their science goals soon after it is deployed.

Argonne anticipates that the new supercomputer will be one of the fastest and most energy-efficient supercomputers in the world after its construction and installation are complete, thanks to a combination of innovative new chip designs and extremely efficient water cooling. Last year, the ALCF won an Environmental Sustainability (EStar) award for the innovative energy-efficient cooling it designed for its current system, and Mira is expected to be significantly more power friendly.

Argonne also envisions Mira as a stepping stone to exascale-class computers that will be faster than petascale-class computers by a factor of a thousand. Exascale computing has the potential to address a class of highly complex workloads that have been beyond our reach, not just due to their sheer size, but because of their inherent uncertainties and unpredictability — challenges like understanding the impacts of regional climate change and the design of safe nuclear reactors.

Mira will offer an opportunity for scientists to become more familiar with the capabilities an exascale machine will offer and the programming changes it will require. For example, it will provide a platform for scaling current computer codes to more than 750,000 individual computing cores and exploring thread-oriented programming, providing them with preliminary experience on how scalability might be achieved on an exascale-class system with hundreds of millions of cores.

Milestones

- The Blue Gene/Q, named Mira, successfully passed several critical decision points (CD-1 and CD-2a in 2009, CD-2b and CD-3 in 2010) in the Department of Energy's (DOE) Independent Project Review.
- A contract was signed to deliver the Blue Gene/Q to the ALCF in the 2012 timeframe.
- The majority of facility enhancements for the Blue Gene/Q were completed.
- ALCF selected and began activities on 16 Early Science projects that will run on the Blue Gene/Q. The ALCF and IBM are providing assistance on the projects. The projects will help shake out the system and software stack using real applications and addressing real science problems.

Once Mira is in production, the DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) and the ASCR Leadership Computing Challenge (ALCC) programs will award blocks of computing time via a peer-reviewed, competitive process to researchers who are working on scientific challenges that are best addressed by the capabilities of high-performance supercomputers.

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PUBLICATIONS

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2010 ALCF Publications

More than 100 publications featured research that was conducted using ALCF resources in 2010.

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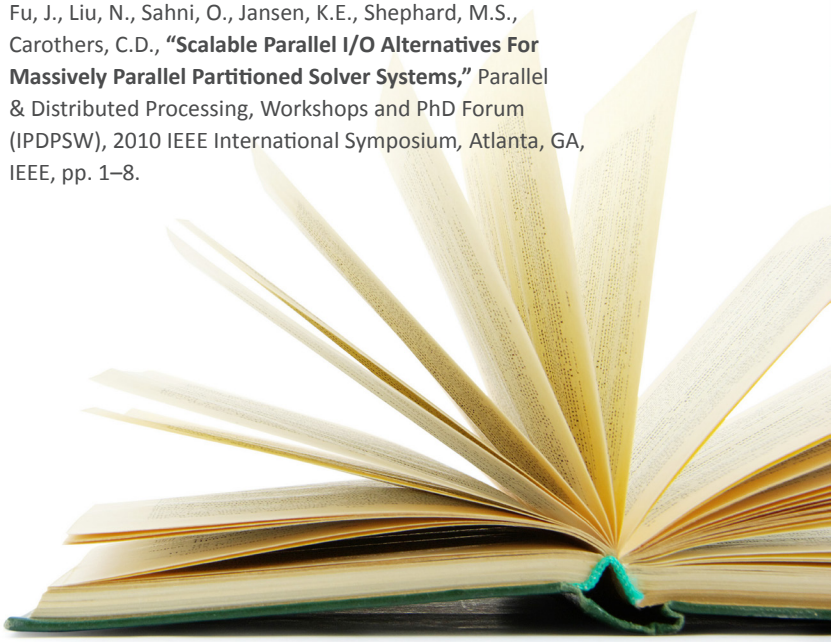

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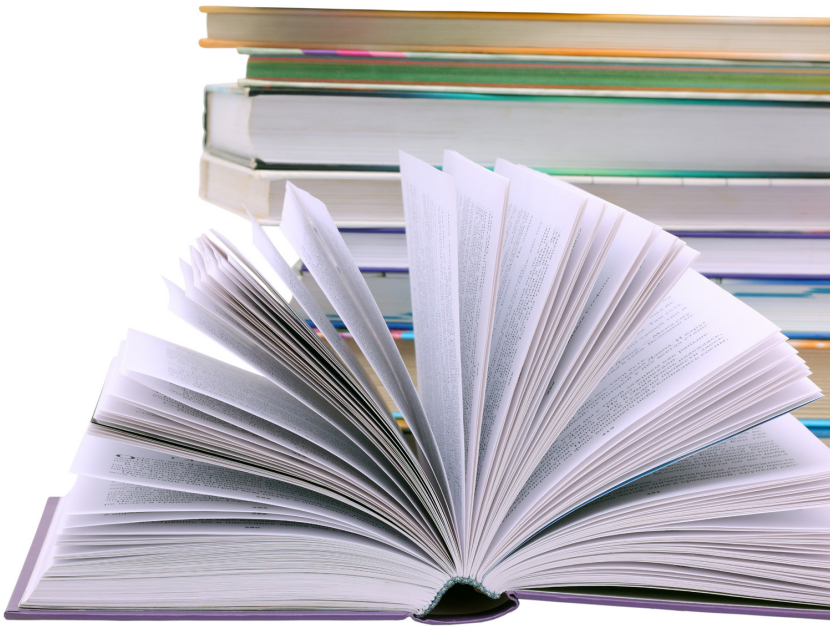


APPENDICES

SCIENCE POWERED BY SUPERCOMPUTING

2010 ANNUAL REPORT

ALCF Research Addresses Critical Grand Challenges in 2010

With U.S. Department of Energy (DOE) support, scientists at the Argonne Leadership Computing Facility (ALCF) gain knowledge of critical global issues at unprecedented scales of time and space — from nanoseconds to decades and from single atoms to global weather systems and supernovae. The scope and precision of this work is immensely demanding. Without powerful computers and precise programming, many computer simulations would take literally decades to run. DOE has long recognized that development of high-performance computers, such as the nimble Intrepid at the ALCF; the networks to connect them; and the software to run them is crucial to America's research lead.

In 2010, researchers received more than 1.11 billion hours of computing time to address grand challenges in a wide array of scientific disciplines at the ALCF. These allocations were awarded through four initiatives — the Innovative and Novel Computational Impact on Theory and Experiment (INCITE), ASCR Leadership Computing Challenge (ALCC), Early Science, and Director's Discretionary programs all provided avenues for conducting transformative science.

Astrophysics

Computational Cosmology
Director's Discretionary Intrepid Allocation: 300,000 Hours

Cosmic Structure Probes of the Dark Universe
Early Science Program Intrepid Allocation: 6 Million Hours

Exploring the Nature of Cold Fronts in Merging Clusters of Galaxies with the FLASH Code
Director's Discretionary Intrepid Allocation: 3.2 Million Hours

FLASH and Supernova Models Project
Director's Discretionary Intrepid Allocation: 100,000 Hours

How Do Standard Candles Illuminate Knowledge of the Universe?
INCITE Program Intrepid Allocation: 70 Million Hours

Petascale Simulations of Turbulent Nuclear Combustion
Early Science Program Intrepid Allocation: 5 Million Hours

Scaling Studies of the MAESTRO and CASTRO Codes on Blue Gene/P
Director's Discretionary Intrepid Allocation: 200,000 Hours

3D Core-Collapse Supernova Simulations
Director's Discretionary Intrepid Allocation: 500,000 Hours

Biological Sciences

Atomistic and Coarse-Grained Molecular Dynamics Simulations of Model Biological Membranes
Director's Discretionary Intrepid Allocation: 2.867 Million Hours

Brain Blood Flow Simulations
Director's Discretionary Intrepid Allocation: 250,000 Hours

Computer-Aided Design of Vaccine Nanoparticles
Director's Discretionary Intrepid Allocation: 500,000 Hours

Fine-Grain Parallelization of UNRES Code for Real-Time Simulations of Large Protein Systems
Director's Discretionary Intrepid Allocation: 100,000 Hours

Gating Mechanisms of Membrane Proteins
Director's Discretionary Intrepid Allocation: 3.918 Million Hours

How Do Researchers Predict the Structures of Biologically Important Proteins?
INCITE Program Intrepid Allocation: 50 Million Hours

HTC-Linux Loosely-Coupled Science Applications
Director's Discretionary Intrepid Allocation: 5 Million Hours

JGI-Pilot Project
Director's Discretionary Intrepid Allocation: 1 Million Hours

Load Balance Spike Communication in Large-Scale Neural Networks
Director's Discretionary Intrepid Allocation: 770,000 Hours

Mesoscale Simulation of Nanoflow and Surface Properties of Amorphous Materials
Director's Discretionary Intrepid Allocation: 100,000 Hours

Modeling the Molecular Basis of Parkinson's Disease
INCITE Program Intrepid Allocation: 5 Million Hours

Multi-Scale Hemodynamics
Director's Discretionary Intrepid Allocation: 2.75 Million Hours

Multi-Scale Molecular Simulations
Director's Discretionary Intrepid Allocation: 5 Million Hours

Multi-Scale Molecular Simulations at the Petascale
Early Science Program Intrepid Allocation: 7.5 Million Hours

Multi-Scale Simulations in Biology: Evolution and Ecology of Microbes
Director's Discretionary Intrepid Allocation: 100,000 Hours

NAMD — The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field
Early Science Program Intrepid Allocation: 7.5 Million Hours
Director's Discretionary Intrepid Allocation: 7.5 Million Hours

Parallel Multi-Objective Optimization Algorithm for de Novo Ligand Design
Director's Discretionary Intrepid Allocation: 2 Million Hours

Protein-Ligand Interaction Simulations and Analysis
Director's Discretionary Intrepid Allocation: 250,000 Hours

Chemistry

Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC
Early Science Program Intrepid Allocation: 7.5 Million Hours

Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow
Director's Discretionary Intrepid Allocation: 5 Million Hours

DNS Simulations of High-Speed Combustion and Detonations
Director's Discretionary Intrepid Allocation: 300,000 Hours

Fragment Molecular Orbital Calculations on Blue Gene/P
Director's Discretionary Intrepid Allocation: 1 Million Hours

High-Accuracy Predictions of the Bulk Properties of Water
Early Science Program Intrepid Allocation: 2 Million Hours

High-Speed Combustion and Detonation (HSCD)
Director's Discretionary Intrepid Allocation: 5 Million Hours

High-Speed Combustion and Detonation (HSCD)
Early Science Program Intrepid Allocation: 5 Million Hours

Ion Permeation through Membranes
Director's Discretionary Intrepid Allocation: 26 Million Hours

Open Protein Simulator
Director's Discretionary Intrepid Allocation: 5 Million Hours

Performing the Largest Unstructured Large Eddy Simulation of a Real, Full Combustion Chamber
INCITE Program Intrepid Allocation: 8 Million Hours

Port ACES and SIAL
Director's Discretionary Intrepid Allocation: 1 Million Hours

Post-Translational Modification Analysis
Director's Discretionary Intrepid Allocation: 2 Million Hours

Predicting Bulk Properties of Water Systems
INCITE Program Intrepid Allocation: 8 Million Hours

Simulation of Large Conformational Transitions in Macromolecular Systems Using Leadership Computing
ALCC Program Intrepid Allocation: 28.5 Million Hours

Testing and Tuning NWChem for Blue Gene/P and Studies of Nonlinear Optical Properties of Conjugated Chromophores
Director's Discretionary Intrepid Allocation: 2 Million Hours

Computer Science and Mathematics

Charm++ and Its Applications
Director's Discretionary Intrepid Allocation: 850,000 Hours

Common Component Architecture Software
Director's Discretionary Intrepid Allocation: 20,000 Hours

Enabling Petascale Science on BG/Q: Tools, Libraries, Programming Models, & Other System Software
Director's Discretionary Intrepid Allocation: 5 Million Hours

Fathom: Geometry, Mesh Generation, and Related Technologies
Director's Discretionary Intrepid Allocation: 100,000 Hours

Graph500 Benchmark Run on Intrepid
Director's Discretionary Intrepid Allocation: 1 Million Hours

Implementing the TotalView Debugger on the ALCF's Blue Gene/P
Director's Discretionary Intrepid Allocation: 5,000 Hours

Improved Debugging Memory Usage for Blue Gene/P
Director's Discretionary Intrepid Allocation: 500,000 Hours

I/O Forwarding Scalability Layer
Director's Discretionary Intrepid Allocation: 1.5 Million Hours

Systems Software Research and Development for ALCF
Director's Discretionary Intrepid Allocation: 3 Million Hours

Parallel Run-Time Systems
Director's Discretionary Intrepid Allocation: 1 Million Hours

PhastaIO: Massively Parallel I/O Experiments of the Phasta CFD Solver
Director's Discretionary Intrepid Allocation: 1 Million Hours

Repast SC++: A Platform for Large-Scale Agent-Based Modeling
Director's Discretionary Intrepid Allocation: 76,800 Hours

TotalView Debugger on Blue Gene/P
Director's Discretionary Intrepid Allocation: 5,000 Hours

Trace Collection for Simulator Driven Codesign of Exascale Platforms and Codes
Director's Discretionary Intrepid Allocation: 500,000 Hours

UltraVis Institute Research for Extreme Scale Visualization
Director's Discretionary Intrepid Allocation: 750,000 Hours

Visualization and Analysis Research and Development for ALCF
Director's Discretionary Intrepid Allocation: 50,000 Hours

ZeptoOS Project
Director's Discretionary Intrepid Allocation: 1 Million Hours

Earth Sciences

A Proposal from the Geophysical Fluid Dynamics Laboratory to Perform Prototype Ultra High-Resolution Climate-Weather Modeling Studies at Argonne National Laboratory
ALCC Program Intrepid Allocation: 25 Million Hours

Assessing Future Hurricane Impacts
Director's Discretionary Intrepid Allocation: 17 Million Hours

CHiMES: Coupled High-Resolution Modeling of the Earth System
Director's Discretionary Intrepid Allocation: 3.475 Million Hours

Climate Modeling Uncertainty Quantification
Director's Discretionary Intrepid Allocation: 200,000 Hours

Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model
Early Science Program Intrepid Allocation: 7.5 Million Hours

How Can More Intricate Climate Models Help Curb Global Warming?
INCITE Program Intrepid Allocation: 30 Million Hours

Large-Scale Hurricane Simulations
Director's Discretionary Intrepid Allocation: 500,000 Hours

Oil Transport Analysis
Director's Discretionary Intrepid Allocation: 2 Million Hours

Scalability of High-Resolution Climate Dynamics
Director's Discretionary Intrepid Allocation: 100,000 Hours

Sensitivity and Uncertainty of Precipitation of the GFDL High-Resolution Model
Director's Discretionary Intrepid Allocation: 100,000 Hours

Using Multi-Scale Dynamic Rupture Models to Improve Ground Motion Estimates
Early Science Program Intrepid Allocation: 7.5 Million Hours

Engineering

A Center for Turbulence Research — Argonne Leadership Computing Facility Collaboratory for Very Large Scale Turbulence Simulations on Petascale Computing Platforms
ALCC Program Intrepid Allocation: 50 Million Hours

Aerodynamics Exploration for Advanced Aero-Propulsion Technologies
ALCC Program Intrepid Allocation: 4.5 Million Hours

Delivering "Green" Low-Noise-Emission Wind Turbines and Jet Engines
INCITE Program Intrepid Allocation: 19 Million Hours

Employing Improved Delayed Detached Eddy Simulations for Turbulent Flows over Tandem Cylinders
Director's Discretionary Intrepid Allocation: 11 Million Hours

Global Simulation of Plasma Microturbulence at the Petascale and Beyond
Early Science Program Intrepid Allocation: 7.5 Million Hours

High Fidelity Direct Noise Prediction for Energy and Propulsion Systems
Director's Discretionary Intrepid Allocation: 10 Million Hours

Improved Boeing IDDES: Delayed Detached Eddy Simulation (IDDES) of Turbulent Flow over a Generic Aircraft Landing Gear
Director's Discretionary Intrepid Allocation: 10 Million Hours

The Interactions between Vaporizing Liquid Droplets and a Turbulent Flow: Fully Resolved DNS
Director's Discretionary Intrepid Allocation: 3 Million Hours

Large Eddy Simulation of Turbulent Mixing by Rayleigh-Taylor Instability
Director's Discretionary Intrepid Allocation: 2 Million Hours

Lattice Boltzmann Simulations for Fluids
Director's Discretionary Intrepid Allocation: 1 Million Hours

Multiphase Mixing Simulations Using the Implicit Lattice Kinetics Method
Director's Discretionary Intrepid Allocation: 200,000 Hours

NEK5000
Director's Discretionary Intrepid Allocation: 4 Million Hours

Performance Analysis of a Low-Mach Number Combustion Code
Director's Discretionary Intrepid Allocation: 500,000 Hours

Petascale, Adaptive CFD
Early Science Program Intrepid Allocation: 2 Million Hours

Petascale Direct Numerical Simulations of Turbulent Channel Flow
Early Science Program Intrepid Allocation: 5 Million Hours

Quantum Lattice Algorithm for Quantum Turbulence
Director's Discretionary Intrepid Allocation: 3.5 Million Hours

Studying Turbulence Using Numerical Simulation
Director's Discretionary Intrepid Allocation: 4 Million Hours

Testing TELEMAC on Intrepid
Director's Discretionary Intrepid Allocation: 340,000 Hours

Materials Science

Algorithms, Codes and Data Analysis in Quantum Simulations of Materials for Energy Applications
Director's Discretionary Intrepid Allocation: 5 Million Hours

Hierarchical Petascale Simulation Framework for Stress Corrosion Cracking
Director's Discretionary Intrepid Allocation: 2 Million Hours

Interpreting IR Stretching Band of Liquid Water Improves Understanding of Hydrogen Bonding
INCITE Program Intrepid Allocation: 1 Million Hours

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Conducting a Large-Scale MD Study of Clay-Polymer Nanocomposites
INCITE Program Intrepid Allocation: 40 Million Hours

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Identifying UPOs in the Navier-Stokes Equations with HYPO4D
INCITE Program Intrepid Allocation: 40 Million Hours

Large-Scale Condensed Matter and Fluid Dynamics Simulations: Simulating Brain Blood Flow to Better Diagnose, Treat Aneurysms
INCITE Program Intrepid Allocation: 40 Million Hours

Materials Design and Discovery: Catalysis and Energy Storage
Early Science Program Intrepid Allocation: 3 Million Hours

Materials Design from First Principles Calculations
Director's Discretionary Intrepid Allocation: 5 Million Hours

Materials Design from First Principles
ALCC Program Intrepid Allocation: 20 Million Hours

Modeling Nickel Fractures and Next-Generation Reactors
Director's Discretionary Intrepid Allocation: 5 Million Hours

Optimization of Real-Space, PAW-Based DFT Codes for Use on the Blue Gene/P
Director's Discretionary Intrepid Allocation: 250,000 Hours

Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
INCITE Program Intrepid Allocation: 10 Million Hours

Using Quantum Chemistry to Study Photocathodes
Director's Discretionary Intrepid Allocation: 0.5 Million Hours

Nuclear Physics

Ab-initio Reaction Calculations for Carbon-12
Early Science Program Intrepid Allocation: 7.5 Million Hours

Advancing the Understanding of Nuclear Structure
INCITE Program Intrepid Allocation: 15 Million Hours

Community Petascale Project for Accelerator Science and Simulation Codes on Blue Gene/P
Director's Discretionary Intrepid Allocation: 1 Million Hours

Direct Multi-Objective Optimization of Storage Ring Lattices for the APS Upgrade and Beyond
ALCC Program Intrepid Allocation: 36 Million Hours

Electromagnetics
Director's Discretionary Intrepid Allocation: 1 Million Hours

Electron Acceleration in Laser Wakefields with High Numerical Resolution
Director's Discretionary Intrepid Allocation: 4 Million Hours

First-Principles Calculation of Laser-Induced Ultrafast Magnetism
Director's Discretionary Intrepid Allocation: 1 Million Hours

How Can We Better Understand the Basic Building Blocks of Nature?
INCITE Program Intrepid Allocation: 67 Million Hours

Improving Light Water Reactor Fuel Reliability Via Flow-Induced Vibration Simulations
ALCC Program Intrepid Allocation: 75 Million Hours

Large-Scale Beam Dynamics Optimization for More Efficient Operation of Large User Facilities
Director's Discretionary Intrepid Allocation: 5 Million Hours

Lattice QCD — Director's Discretionary
Director's Discretionary Intrepid Allocation: 5 Million Hours

Lattice Quantum Chromodynamics
Early Science Program Intrepid Allocation: 7.5 Million Hours

Nucleon Structure Down to the Physical Pion Mass
ALCC Program Intrepid Allocation: 37.8 Million Hours

Optimization on Nonlinear Dynamics for the APS Upgrade
Director's Discretionary Intrepid Allocation: 1 Million Hours

Petascale Computational Accelerator Physics
Director's Discretionary Intrepid Allocation: 6 Million Hours

Petascale Simulations of Turbulent Nuclear Combustion
Director's Discretionary Intrepid Allocation: 5 Million Hours

Pion Mass
Director's Discretionary Intrepid Allocation: 38 Million Hours

RERTR Project
Director's Discretionary Intrepid Allocation: 300,000 Hours

Scalable, Explicit Geometry, Whole-Core Nuclear Reactor Simulations
ALCC Program Intrepid Allocation: 38 Million Hours

Scalable Simulation of Neutron Transport in Fast Reactor Cores
Director's Discretionary Intrepid Allocation: 250,000 Hours

Studies in Magnetohydrodynamic Turbulence
Director's Discretionary Intrepid Allocation: 400,000 Hours

Plasma Physics

Advanced 2D and 3D Laser-Produced and Electrically Driven Plasma Processes Modeling for EUV Lithography and Other Advanced Plasma Applications
Director's Discretionary Intrepid Allocation: 300,000 Hours

Exploring Particle-in-Cell/Hybrid Simulations of Fast Ignition
INCITE Program Intrepid Allocation: 7 Million Hours

FACETS
Director's Discretionary Intrepid Allocation: 500,000 Hours

Performance Studies of the IMPACT-Z Parallel Particle-in-Cell Accelerator Modeling Code
Director's Discretionary Intrepid Allocation: 100,000 Hours

Simulating Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond
INCITE Program Intrepid Allocation: 45 Million Hours

2011 INCITE Research Projects

In 2011, 30 projects in diverse scientific disciplines were awarded approximately 732 million supercomputer core-hours on the Blue Gene/P at the ALCF through the Department of Energy's INCITE (Innovative and Novel Computational Impact on Theory and Experiment) Program. Of these, 12 projects were renewed from 2010, and 18 are new projects.

Biological Sciences

Multiscale Blood Flow Simulations
George Karniadakis, Brown University
Intrepid Allocation: 50,000,000 Hours

Protein-Ligand Interaction Simulations and Analysis
T. Andrew Binkowski, Argonne National Laboratory
Intrepid Allocation: 20,000,000 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: 4,000,000 Hours

Chemistry

Towards Breakthroughs in Protein Structure Calculation and Design
David Baker, University of Washington
Intrepid Allocation: 30,000,000 Hours

Simulations of Deflagration-to-Detonation Transition in Reactive Gases
Alexei Khokhlov, University of Chicago
Intrepid Allocation: 18,000,000 Hours

Potential Energy Surfaces for Simulating Complex Chemical Processes
Donald Truhlar, University of Minnesota
Intrepid Allocation: 15,000,000 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: 10,000,000 Hours

Ab Initio Dynamical Simulations for the Prediction of Bulk Properties
Theresa Windus, Iowa State University
Intrepid Allocation: 10,000,000 Hours

Computer Science

Performance Evaluation and Analysis Consortium End Station
Patrick Worley, Oak Ridge National Laboratory
Intrepid Allocation: 10,000,000 Hours

Scalable System Software for Performance and Productivity
Ewing Lusk, Argonne National Laboratory
Intrepid Allocation: 5,000,000 Hours

Trace Collection for Simulation-driven Co-design of Exascale Platforms and Codes
David Evensky, Sandia National Laboratory
Intrepid Allocation: 5,000,000 Hours

Earth Science

Climate-Science Computational Development Team: The Climate End Station II
Warren Washington, National Center for Atmospheric Research
Intrepid Allocation: 40,000,000 Hours

Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence
Susan Kurien, Los Alamos National Laboratory
Intrepid Allocation: 35,000,000 Hours

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz
Thomas Jordan, University of Southern California
Intrepid Allocation: 10,000,000 Hours

Energy Technologies

Advanced Reactor Thermal Hydraulic Modeling
Paul Fischer, Argonne National Laboratory
Intrepid Allocation: 25,000,000 Hours

Large Eddy Simulation for Green Energy and Propulsion Systems
Umesh Paliath, GE Global Research
Intrepid Allocation: 20,000,000 Hours

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air
Jack Wells, Oak Ridge National Laboratory
Intrepid Allocation: 15,000,000 Hours

Engineering

Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders
Philippe Spalart, Boeing
Intrepid Allocation: 45,000,000 Hours

Simulation of High Reynolds Number Turbulent Boundary Layers
Robert Moser, University of Texas at Austin
Intrepid Allocation: 40,000,000 Hours

Turbulent Multi-material Mixing in the Richtmyer-Meshkov Instability
Sanjiva Lele, Stanford University
Intrepid Allocation: 12,000,000 Hours

Uncertainty Quantification for Turbulent Mixing
James Glimm, State University of New York, Stony Brook
Intrepid Allocation: 10,000,000 Hours

Materials Science

Petascale Simulations of Stress Corrosion Cracking
Priya Vashishta, University of Southern California
Intrepid Allocation: 45,000,000 Hours

High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry
William George, National Institutes of Standards and Technology
Intrepid Allocation: 25,000,000 Hours

Probing the Non-scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
Jeffrey Greeley, Argonne National Laboratory
Intrepid Allocation: 15,000,000 Hours

Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces
Giulia Galli, University of California–Davis
Intrepid Allocation: 15,000,000 Hours

Physics

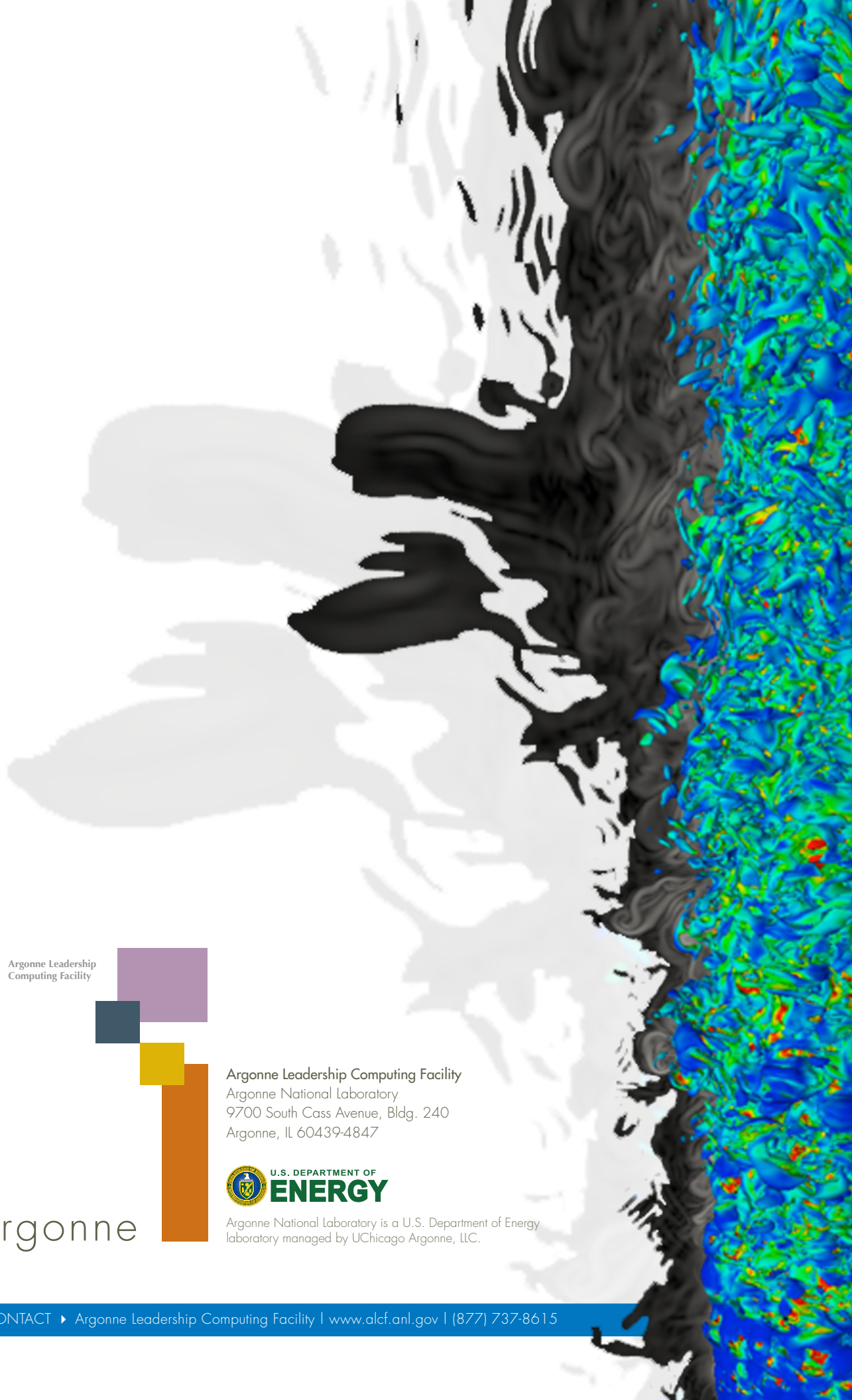
Study of Buoyancy-driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models
Donald Lamb, The University of Chicago
Intrepid Allocation: 80,000,000 Hours

Lattice QCD
Paul Mackenzie, Fermi National Accelerator Laboratory
Intrepid Allocation: 50,000,000 Hours

Simulations of Laser-plasma Interactions in Targets for the National Ignition Facility and Beyond
Denise Hinkel, Lawrence Livermore National Laboratory
Intrepid Allocation: 50,000,000 Hours

Nuclear Structure and Nuclear Reactions
James Vary, Iowa State University
Intrepid Allocation: 15,000,000 Hours

Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond
William Tang, Princeton Plasma Physics Laboratory
Intrepid Allocation: 8,000,000 Hours



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