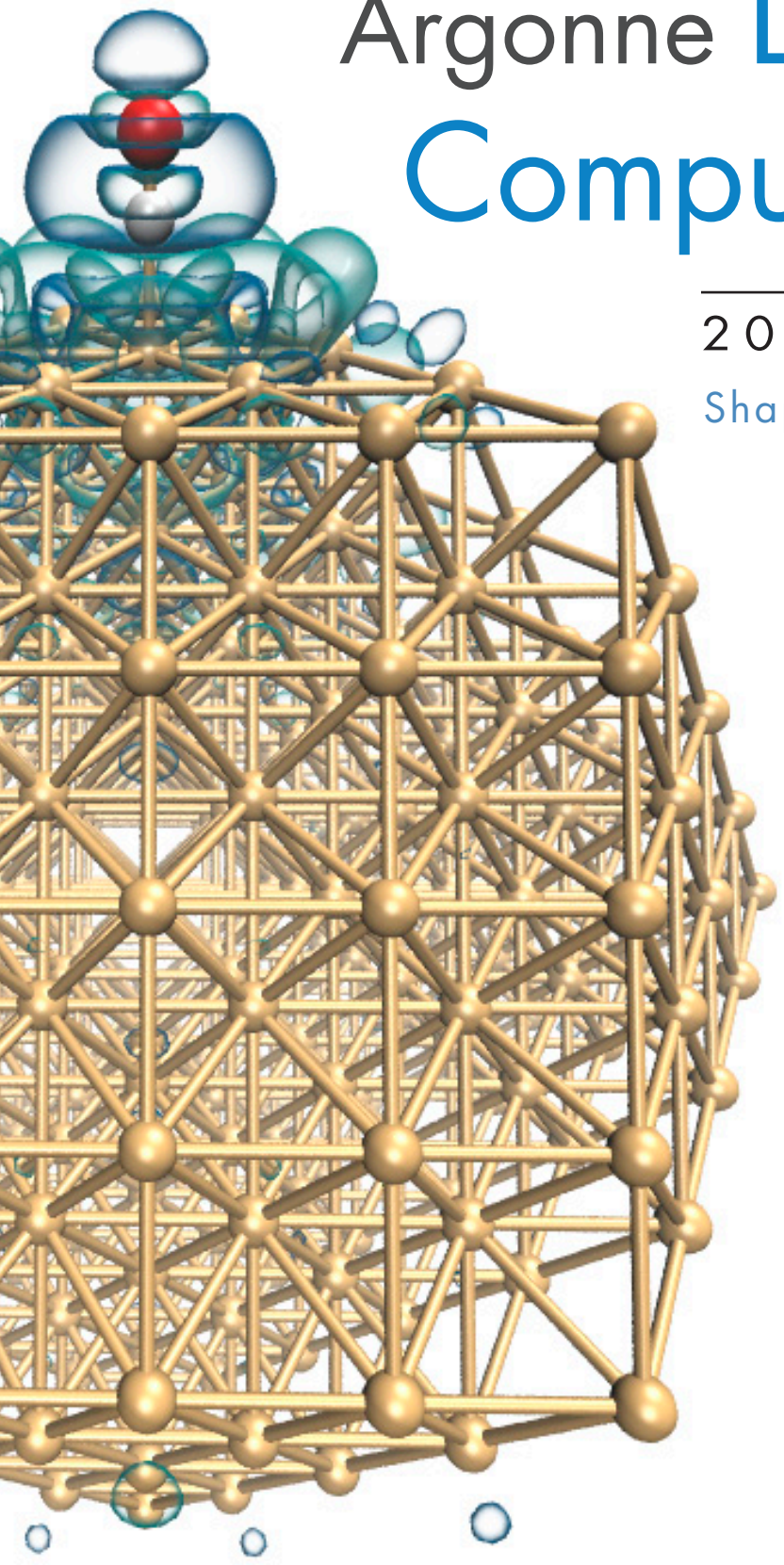
ANL-12/22

Argonne Leadership Computing Facility

2011 annual report

Shaping Future Supercomputing



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Argonne Leadership Computing Facility

2011 alcf annual report
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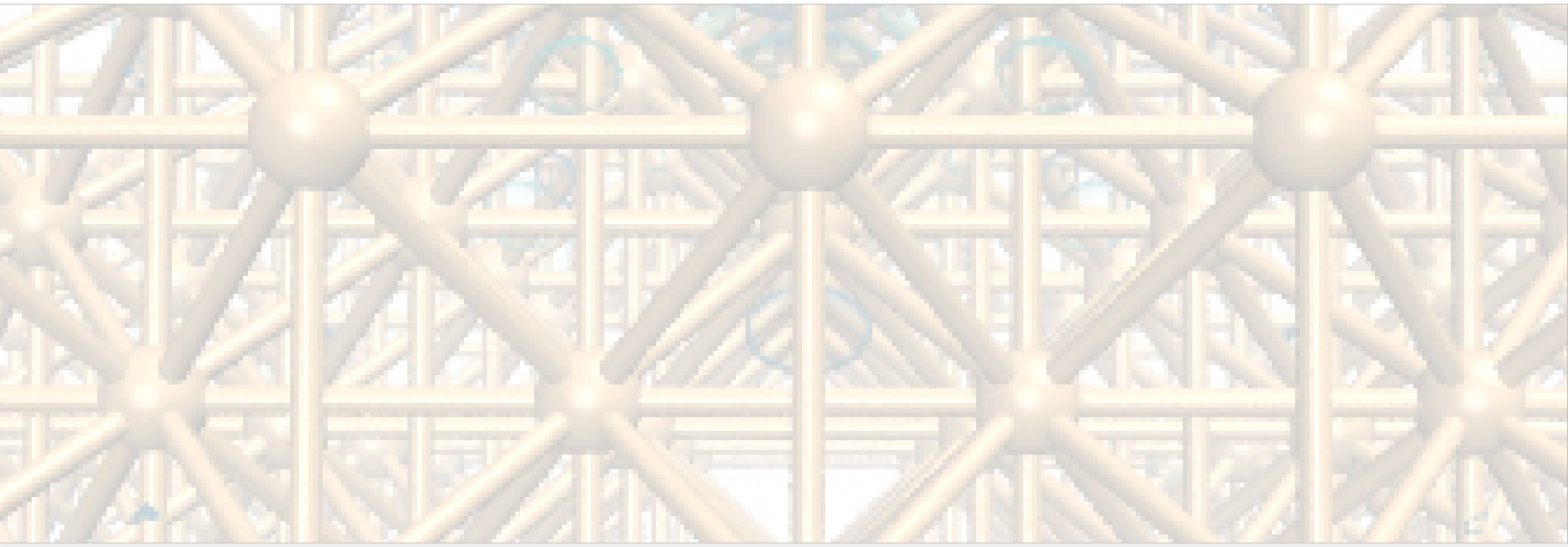

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On the cover

This image shows the charge density difference of a carbon monoxide molecule adsorbed (adhered to the surface) of a 309-atom gold naoparticle. Gold, oxygen, and carbon atoms are colored gold, red, and white, respectively. The blue translucent isosurface depicts charge density depletion, and the green translucent isosurface depicts charge density accumulation.
Image credit: "Finite Size Effects in Chemical Bonding: From Small Clusters to Solids," Catalysis Letters, Vol. 141, No. 8, June 2011, pp. 1067-1071.
Image rendered by Joe Insley, Argonne National Laboratory.

Shaping the Future of Supercomputing with Mira

With great anticipation, we've been preparing for the arrival of Mira, the 10-petaflops IBM Blue Gene/Q system that will be 20 times faster than Intrepid, the Blue Gene/P, our current machine, and the greenest supercomputer in the world. (It topped supercomputing's Green 500 list even before it was installed!)

The name "Mira" comes from the Latin words for *wonderful, surprising, remarkable, extraordinary*. It's also similar to the Italian word *mirino*, which means viewfinder. The words reference the discoveries that Mira will enable once the machine is fully up and running.

Like any new arrival, the supercomputer promises to deliver both marvels and challenges. The BG/Q is capable of carrying out 10 quadrillion calculations per second, allowing scientists to tackle larger problems, achieve faster times to solutions, and create more accurate models. It will offer an open source and standards-based programming environment. It will provide a small footprint and ultra-low power consumption. With all these benefits, the system will also present researchers and ALCF staff with the challenges of maximizing its capabilities and performance to produce unequaled scientific breakthroughs.

However, equally compelling challenges have been met successfully on Mira's predecessor—Intrepid, the ALCF's Blue Gene/P system—and tomorrow's strides in scientific supercomputing will build on today's achievements. In 2011, scientists conducted research on a diverse range of key projects that used approximately 1.2 billion core-hours on Intrepid. Dedicated ALCF staff worked hand-in-hand with them to ensure that ALCF resources provided maximum performance. These collaborative efforts resulted in breathtaking scientific results and paved the way for Mira.

To support the science that will be run on Mira, the ALCF team installed 35 petabytes of storage technology in the data center. Two testing and development racks—named Cetus and Vesta—were delivered in early January 2012. Once installed, the first researchers to access them will be those selected through the Early Science Program. In addition, key developers of essential computational tools for users will be given access to the system to complete the process of porting the tools for use on the Blue Gene/Q architecture.

Full production on Mira is expected in 2013. Besides being a star performer in leadership-class computing, Mira will bring us closer to our vision for the future: exascale speed, where computers will calculate quintillions of floating point operations per second. Think how quickly the world's most intractable problems in such critical areas as health, energy, climate, and physics can be addressed with these strides in supercomputing!

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

ALCF Evolution

2004
- Formed the Blue Gene Consortium with IBM

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

2006
- Supported 6 INCITE projects
- Continued code development and evaluation of Blue Gene/L
- Signed contract for Intrepid

2007
- Supported 9 INCITE projects
- Continued development projects
- Held Next-Generation Blue Gene workshop
- Installed 100-teraflops Blue Gene/P
- Accepted 100-teraflops Blue Gene/P

2008
- Supported 20 INCITE projects
- Dedicated the ALCF in April
- Intrepid named world's fastest supercomputer for open science
- Installed Eureka, providing a quantum leap in visualization

2009
- Brought the 557-teraflops Intrepid into full production
- Supported 28 INCITE projects
- Delivered more than 1 million core-hours of science

2010
- Supported 35 INCITE projects and 10 ALCC projects
- Signed contract for Mira, the next-generation Blue Gene/Q supercomputer
- Selected 16 Early Science Program (ESP) projects to run on the 10-petaflops Mira
- Delivered more than 2 billion core-hours of science since the ALCF's inception

2011
- Supported 30 INCITE, 7 ALCC, and 16 ESP projects
- Signed contract for delivery of Mira to the ALCF in 2012
- Planned facility enhancements completed for Mira
- Prepared for Tukey, which will be twice as fast as its predecessor, Eureka
- Delivered 1.2 billion core-hours of science

ALCF: Leadership-Class Computing for Pioneering Science

The Argonne Leadership Computing Facility (ALCF) is one of two leadership computing facilities supported by the U.S. Department of Energy (DOE). The ALCF provides the computational science community with a world-class computing capability dedicated to groundbreaking science and engineering. It began operation in 2006 with its team providing expertise and assistance to support user projects to achieve top performance of applications and to maximize benefits from the use of ALCF resources.

Enabling Science

In 2011, the ALCF's 1.2 billion core-hours were devoted to such worthy research endeavors as explorations into renewable energy, studies of the effects of global climate change, and efforts to unravel the origins of the universe.

Mission and Vision

The ALCF's 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.

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.

Accelerating Transformational Discovery

High-performance computing is becoming increasingly important as more scientists and engineers use modeling and simulation to study intricate chemical processes, exotic new materials, advanced energy networks, natural ecosystems, and sophisticated energy technologies. One of the world's fastest computers for open science, Intrepid, Argonne's IBM Blue Gene/P, is capable of more than 500 trillion calculations per second. By 2013, Mira—an IBM Blue Gene/Q supercomputer capable of running programs at 10 quadrillion calculations per second—will be in full production at the ALCF. It will provide billions more core-hours each year to researchers worldwide for rapidly conducting transformational science.


Blue Gene Q supercomputer

Mira USHERS IN A NEW ERA OF SCIENTIFIC SUPERCOMPUTING

Mira, the new petascale IBM Blue Gene/Q system being installed at the ALCF, will usher in a new era of scientific supercomputing. An engineering marvel, the 10-petaflops machine is capable of carrying out 10 quadrillion calculations per second. To put this speed into perspective: If every single person on earth solved one calculation per second, around the clock, it would take them more than two weeks to do the work that Mira will accomplish in one second!

As computers get faster and more powerful, they also need to get more energy efficient to be practical. Mira will be five times more energy efficient than Intrepid, its Blue Gene/P predecessor at the ALCF. Copper tubes will pipe cold water directly alongside the chips, which saves power by eliminating the extra cooling step. In addition, Mira fits more cores onto a single chip. This arrangement reduces the distance that data has to travel between the chips, which speeds communication between cores and saves the energy lost when transporting data across long distances.

To ensure that science applications will be prepared to run on Mira as soon as possible, ALCF staff is working with 16 research teams from across the nation to port and tune their codes on Blue Gene/Q prototype hardware. This period provides the teams' projects with a significant head start for adapting to the new machine and access to substantial computational time. During this shakedown phase, users assist in identifying the root causes of any system instabilities and work with ALCF staff to help develop solutions. ALCF staff has also been working with the community and vendors through a performance project to ensure that the performance tools, debuggers and libraries, with which they have become familiar on Intrepid, are ported to Mira and available for Early Science users.

These Early Science Program projects cover a range of scientific fields representative of Mira's projected computational workload, including simulations of advanced materials, exploration of the universe, modeling of biological organisms, and the design of new, safe, and reliable sources of energy.

Mira is expected to be in full production in 2013. The remarkable next-generation supercomputer represents a milestone in the ongoing effort to develop exascale systems for open science equipped with hundreds of millions of processors within the decade.

MIRA PROVIDES PETAFLOPS POWER

Mira, the ALCF's next-generation Blue Gene/Q system, will consist of:

- 48 racks
- 1,024 nodes per rack
- 1.6 GHz 16-core processor and 16 GB RAM per node
- 384 I/O nodes
- 240 GB/s, 35PB storage

For a total of 768K cores, 768 terabytes of RAM, and a peak performance of 10 petaflops. The system is capable of carrying out *10 quadrillion floating-point operations per second.*

GETTING A JUMP START WITH EARLY SCIENCE

The ALCF's Early Science Program aims to prepare key applications for the architecture and scale of Mira and to solidify libraries and infrastructure that will pave the way for other future production applications. Two billion core-hours have been allocated to 16 Early Science projects on Mira. The projects, in addition to promising delivery of exciting new science, are all based on state-of-the-art, petascale, parallel applications. The project teams, in collaboration with ALCF staff and IBM, have undertaken intensive efforts to adapt their software to take advantage of Mira's Blue Gene/Q architecture, which, in a number of ways, is a precursor to future high-performance-computing architectures.

Biological Sciences

NAMD—The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field
PI: Benoit Roux, The University of Chicago
80 Million Hours

Multiscale Molecular Simulations at the Petascale
PI: Gregory Voth, The University of Chicago
150 Million Hours

Chemistry

High-Accuracy Predictions of the Bulk Properties of Water
PI: Mark Gordon, Iowa State University
150 Million Hours

Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC
PI: Robert Harrison, Oak Ridge National Laboratory
150 Million Hours

High-Speed Combustion and Detonation (HSCD)
PI: Alexei Khokhlov, The University of Chicago
150 Million Hours

Earth Science

Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model
PI: Venkatramani Balaji, Geophysical Fluid Dynamics Laboratory
150 Million Hours

Engineering

Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow
PI: Christos Frouzakis, Swiss Federal Institute of Technology
150 Million Hours

Petascale, Adaptive CFD
PI: Kenneth Jansen, University of Colorado—Boulder
150 Million Hours

Petascale Direct Numerical Simulations of Turbulent Channel Flow
PI: Robert Moser, University of Texas
60 Million Hours

Geophysics

Using Multi-Scale Dynamic Rupture Models to Improve Ground Motion Estimates
PI: Thomas Jordan, University of Southern California
150 Million Hours

Materials Science

Materials Design and Discovery: Catalysis and Energy Storage
PI: Larry Curtiss, Argonne National Laboratory
50 Million Hours

Physics

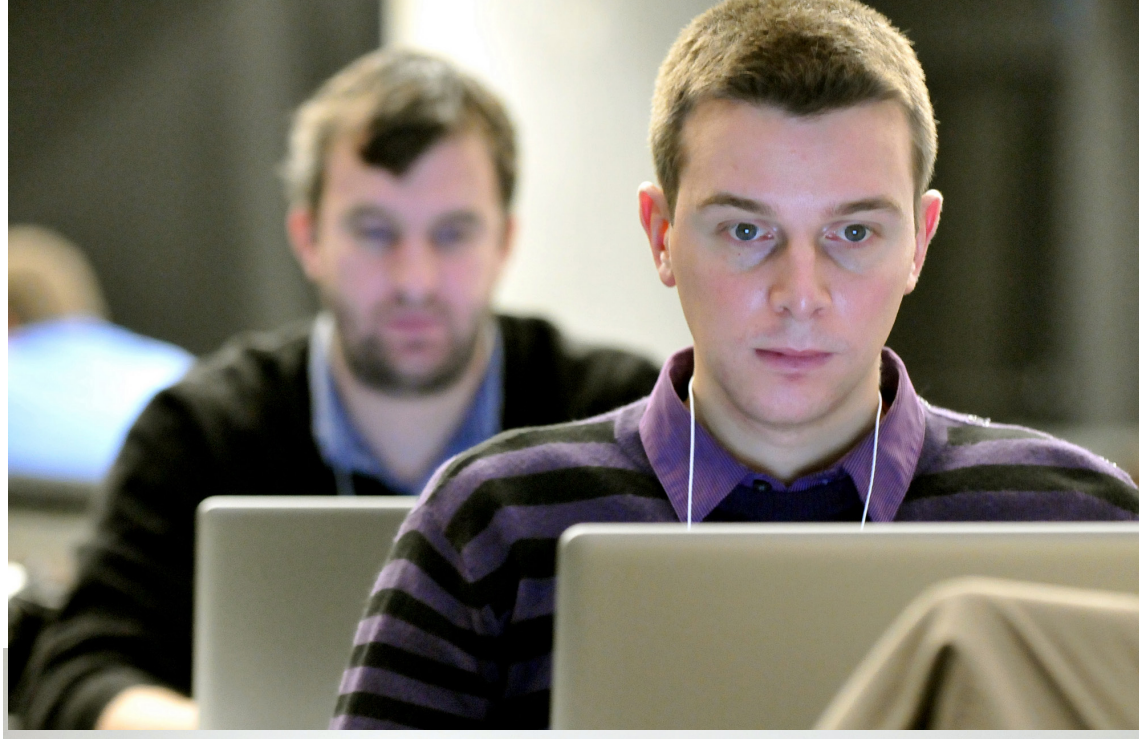
Cosmic Structure Probes of the Dark Universe
PI: Salman Habib, Los Alamos National Laboratory
150 Million Hours

Petascale Simulations of Turbulent Nuclear Combustion
PI: Don Lamb, The University of Chicago
150 Million Hours

Lattice Quantum Chromodynamics
PI: Paul Mackenzie, Fermilab
150 Million Hours

Ab-initio Reaction Calculations for Carbon-12
PI: Steven C. Pieper, Argonne National Laboratory
110 Million Hours

Global Simulation of Plasma Microturbulence at the Petascale and Beyond
PI: William Tang, Princeton Plasma Physics Laboratory
50 Million Hours



SCIENCE HIGHLIGHTS

The Argonne Leadership Computing Facility (ALCF) enables transformative science that solves some of the most difficult challenges in biology, chemistry, energy, climate, materials, physics, and other scientific realms. Users partnering with ALCF staff have reached research milestones previously unattainable, due to the ALCF's world-class supercomputing resources and expertise in computation science.

In 2011, the ALCF's commitment to providing outstanding science and leadership-class resources was honored with several prestigious awards. Research on multiscale brain blood flow simulations was named a Gordon Bell Prize finalist. Intrepid, the ALCF's BG/P system, ranked No. 1 on the Graph 500 list for the second consecutive year. The next-generation BG/Q prototype again topped the Green500 list.

Skilled experts at the ALCF enable researchers to conduct breakthrough science on the Blue Gene system in key ways.

The *Catalyst Team* matches project PIs with experienced computational scientists to maximize and accelerate research in their specific scientific domains.

The *Performance Engineering Team* facilitates the effective use of applications on the Blue Gene system by assessing and improving the algorithms used by applications and the techniques used to implement those algorithms.

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

The *Operations Team* ensures that system hardware and software work reliably and optimally; system tools are matched to the unique system architectures and scale of ALCF resources; the entire system software stack works smoothly together; and I/O performance issues, bug fixes, and requests for system software are addressed.

The *User Services and Outreach Team* offers frontline services and support to existing and potential ALCF users. The team also provides marketing and outreach to users, DOE, and the broader community.

Science Director's Message

Pursuing Groundbreaking Science

The next major computational resource in the ALCF—Mira, the 10-petaflops IBM Blue Gene/Q (BG/Q)—will arrive in 2012. Its powerful configuration, with 48K nodes, 768K cores, and 786 terabytes of memory, may be daunting at first. However, early experience in porting applications to small BG/Q configurations has confirmed that codes running on IBM Blue Gene/P (BG/P) systems require no modifications to run on BG/Q and achieve substantial performance increases over the same number of BG/P nodes. Furthermore, in 2011 just under 50% of the core-hours used on Intrepid, the ALCF's BG/P system, were by long production jobs that ran on 8K-, 16K-, and 32K-node partitions and produced important scientific and engineering results. Such scalability advances and the early experience running on BG/Q hardware bode well for pursuing groundbreaking computational science on Mira.

As we look forward to Mira, we are also drawn to looking back at Argonne's activities in parallel computing. Thirty years ago, Argonne scientists began to investigate algorithms, programming models, and tools for parallel architectures. In 1984 the first system was installed, followed shortly by four other systems of diverse architectures, one of which had as many as 24 processors! Many other parallel computers ensued, providing resources for scientific advances, testbeds for methodologies and software, and a training ground for computational and computer scientists. It is rewarding to learn from eminent scientists that their first exposure to parallel computing occurred at Argonne in the 1980s and that the experience caused a major change in their career. We aim to continue to provide leadership-level computing experiences that cause career swerves.

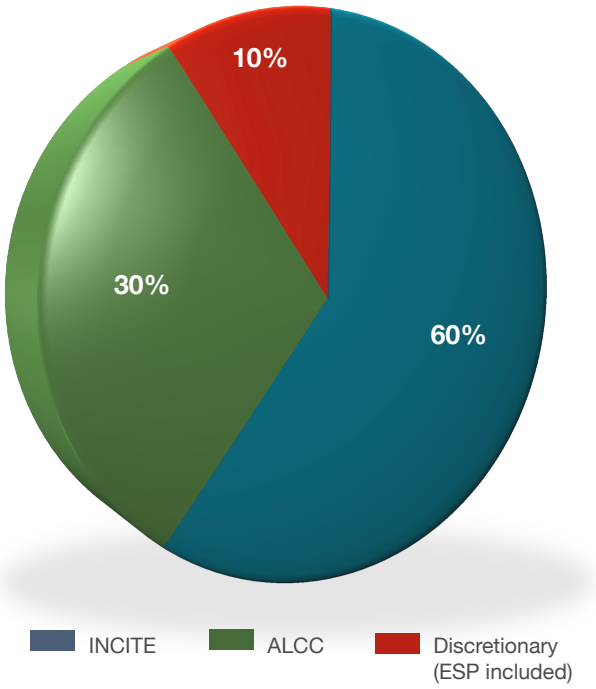
In this report, we describe 22 projects that used Intrepid. It was painful to feature so few. The projects that win allocations on ALCF resources have compelling goals, and the researchers pursue them with skill and dedication. This subset was selected to represent every major application domain and includes projects from all three award categories: INCITE, ALCC, and Director's Discretionary. I hope you will enjoy reading this sampling.

Paul Messina
Director of Science | Argonne Leadership Computing Facility

ALCF Awards Benefit A Wide Array of Users, Challenges

Argonne Leadership Computing Facility (ALCF) staff works closely with researchers from academia, industry, and national laboratories—as well as federal, state, and municipal agencies—to help them solve complex challenges, advance America's scientific leadership, and prepare the nation for a better future.

Access to Intrepid, the IBM Blue Gene/P supercomputer at the ALCF, is available for research primarily through Department of Energy (DOE) Office of Science allocation programs. Approximately 60% percent of ALCF resources are awarded to researchers with computationally intensive, large-scale research projects through DOE's INCITE program. The DOE ASCR Leadership Computing Challenge (ALCC) program allocates 30% of the ALCF's resources for projects of interest to DOE's energy mission. Argonne researchers may also apply for time through the locally managed Director's Discretionary program, a smaller initiative (about 10% of resources) designed to prepare smaller projects for a future INCITE award. Early Science Program projects also tap into this allocation of time.



Percentage of INCITE, ALCC, Director's Discretionary, and Early Science Program (ESP) 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 Oak Ridge 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. Projects are awarded an INCITE allocation based on a peer review for scientific merit and computational readiness. The program 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)

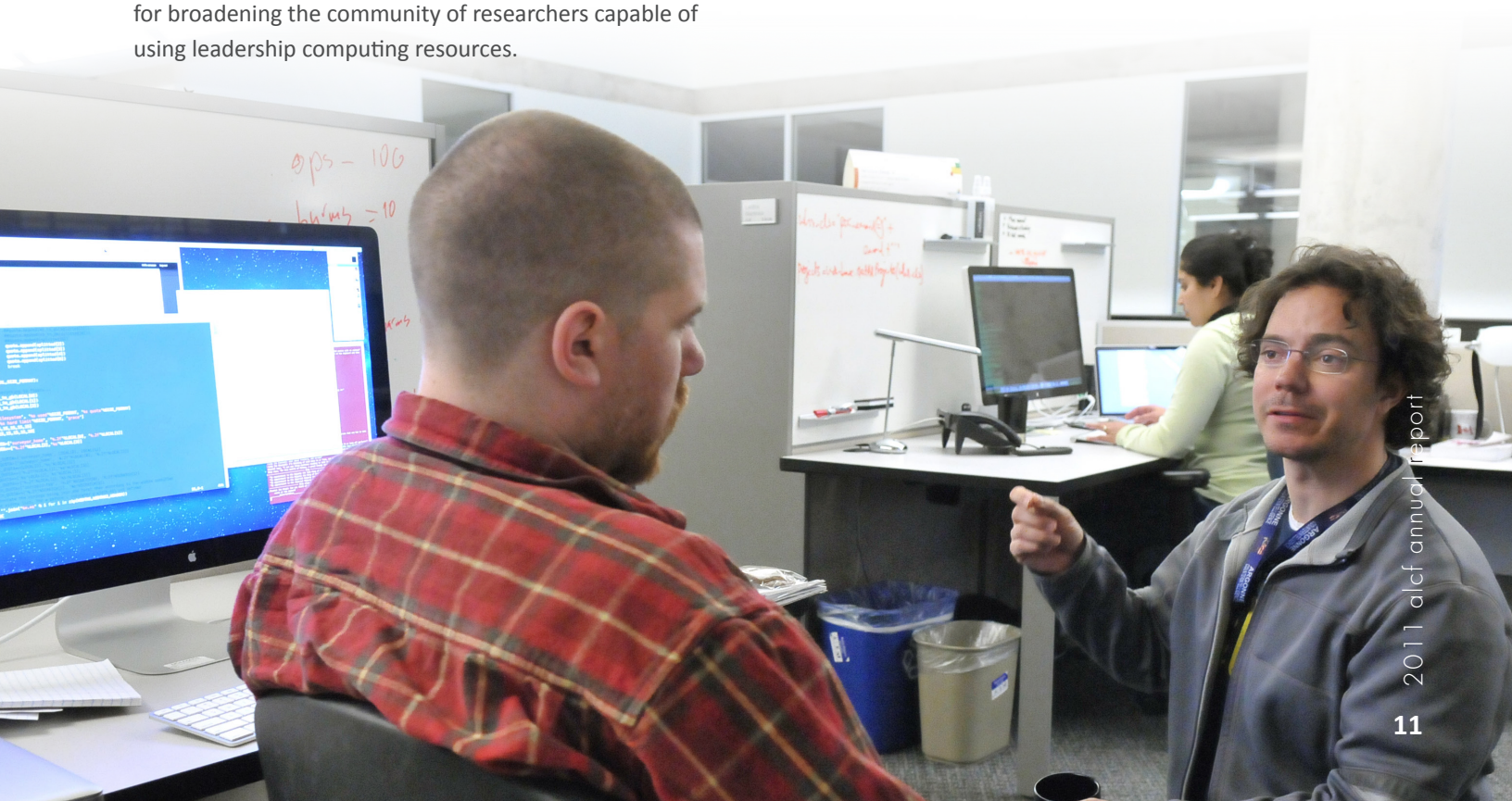
Open to scientists from the research community in academia and industry, the ALCC program allocates resources to projects with an emphasis on high-risk, high-payoff simulations in areas directly related to the Department's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources.

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. Two billion core-hours are allocated through ESP.

Discretionary Projects

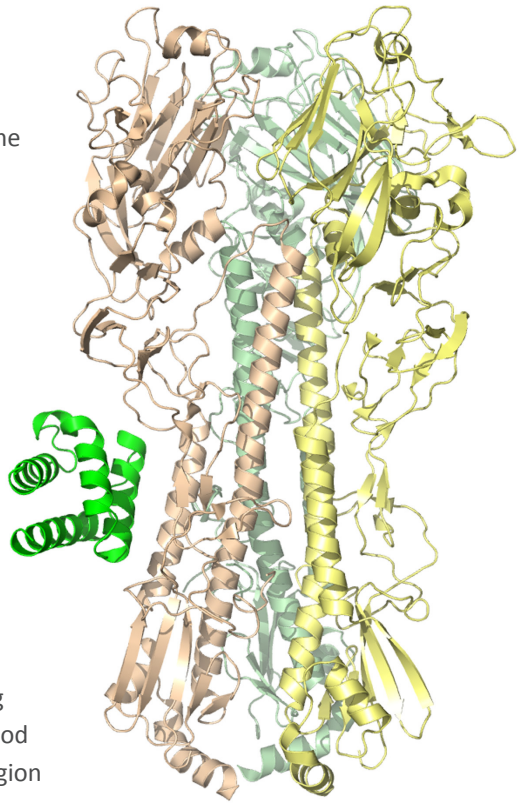
Discretionary allocations are "start up" awards made to potential future INCITE projects so that they can achieve computational readiness. Projects must demonstrate a need for leadership-class resources. Awards may be made year round to industry, academia, laboratories and others, and are usually between 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

Breakthroughs in Protein Structure Calculation and Design

INCITE Allocation: 30 Million Hours
PI: David Baker (dabaker@u.washington.edu) | University of Washington



Protein structure prediction is key to understanding the function and interactions of biomolecules and provides the insights necessary to design new molecules with novel and useful functions. Faster and more accurate predictions of structure can yield significant cost and time savings. In collaboration with other researchers, David Baker from the University of Washington has achieved several exciting breakthroughs in protein structure calculation and design. The researchers developed a new approach for computational analysis of Nuclear Magnetic Resonance (NMR) data that pushes the limits of protein size that can be structurally solved from NMR spectroscopy data. They also invented an approach in which electron density maps generated from molecular replacement solutions for each of a series of starting models are used to guide energy optimization by structure rebuilding, combinatorial side chain packing, and torsion space minimization. In another effort addressing the challenges of influenza, the team devised a computational method for designing protein-protein interactions de novo and used the method to design high-affinity binders to the conserved stem region on influenza hemagglutinin. The results suggest that de novo computational design of antiviral proteins is feasible.

Multiscale Models Offer More Realistic Picture of Brain Blood Flow

INCITE Allocation: 50 Million Hours
PI: George Karniadakis (george_karniadakis@brown.edu) | Brown University

To treat diseases involving disruptions of blood flow to the brain, doctors must first understand how multiple scales of blood vessel networks work within the brain, both alone and together. A research team led by George Karniadakis from Brown University is using ALCF resources to create multiscale models that show the interconnected workings of multiple scales of the brain's blood vessels. The simulations use MRI data of actual patients for generating the geometry and meshes of the vasculature. The team collaborated with the ALCF's Mike Papka and Joe Insley on creating multiscale visualizations of the huge amount of data generated. The research is an extension of an earlier ALCF Discretionary project, in which the runs were conducted for Karniadakis' Gordon Bell submission, which was named a Gordon Bell Prize finalist. Multiscale models provide doctors with a more realistic picture of blood flow, and the greatest hope for the development of new lifesaving treatments for such blood-related diseases as brain aneurysms, sickle-cell anemia, and cerebral malaria.

Chemistry

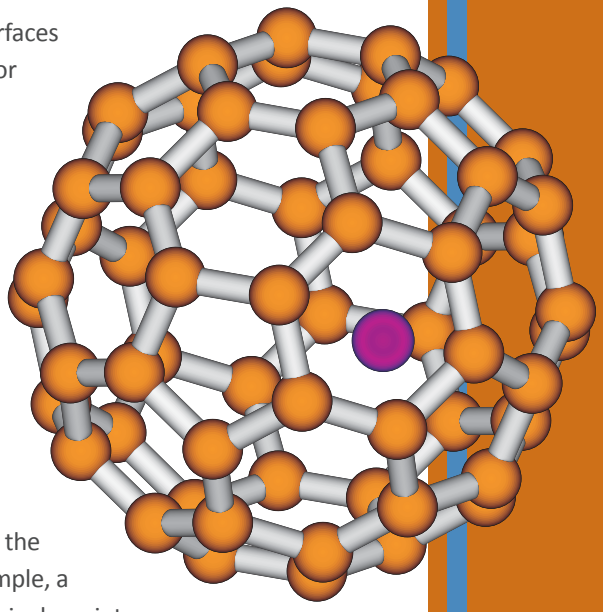
Performing the Largest Unstructured Large-Eddy Simulation of a Real, Full Combustion Chamber

INCITE Allocation: 10 Million Hours
PI: Thierry Poinsot (Thierry.poinsot@cerfacs.fr) | CERFACS

Researchers from CERFACS (the European Centre for Research and Advanced Training in Scientific Computation) have performed top-of-the-line quality simulations on highly complex cases in their goal towards the fully numerical modeling of an actual combustor. Led by Thierry Poinsot, their 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 ALCF leadership-class supercomputer, the researchers have performed the largest unstructured LES done to date of a commercial, 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. 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). Research results are featured in a paper by Pierre Wolf, et al., "Using LES to Study Reacting Flows and Instabilities in Annular Combustion Chambers," *Flow Turbulence & Combustion,* Springer Science & Business Media, published online in September 2011.

Potential Energy Surfaces for Simulating Complex Chemical Processes

INCITE Allocation: 15 Million Hours
PI: Don Truhlar (truhlar@umn.edu) | University of Minnesota

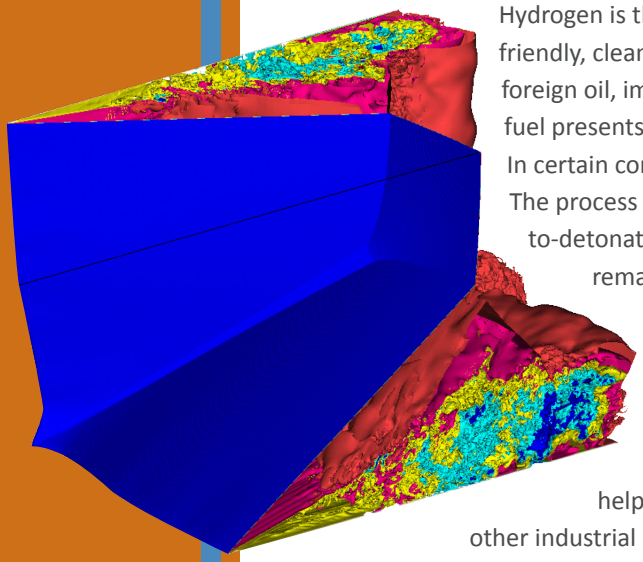


Large-scale electronic structure theory can provide potential energy surfaces and force fields for simulating complex chemical processes important for technology and biological chemistry. During the past year, University of Minnesota researchers carried out calculations to study structural and electronic factors in metallofullerenes and semimetal-fullerenes; the goal is to achieve a deeper understanding of the interactions that are important to their functional use as molecular electronic device components. From both a fundamental, theoretical point of view and a practical one, it is essential to find the energy minima and saddle points of low-lying electronic states and to map the topography of the seams of conical intersections in these fascinating systems.

ALCF staff worked with the project team to improve the performance of the key algorithm, which is the multi-configurational self-consistent field (MCSCF) method in the GAMESS code. This improvement enabled the researchers to perform large-scale calculations very efficiently. For example, a state-averaged complete active space self-consistent field (SA-CASSCF) single-point energy calculation of the Ca@C60 system (the endohedral complex consisting of a single Ca atom inside a "buckyball" fullerene) running on 8,192 cores on Intrepid, the Blue Gene/P supercomputer at the ALCF, takes only ~40 minutes. This time is twice as fast as the same calculation using the standard version of the GAMESS code. This difference is significant when one considers that typically researchers need to run hundreds of such calculations. The researchers expect an even greater improvement in the performance for bigger problems.

Simulations of Deflagration-to-Detonation Transition in Reactive Gases

INCITE Allocation: 18 Million Hours
PI: Alexei Khokhlov (ajk@oddjob.uchicago.edu) | The University of Chicago



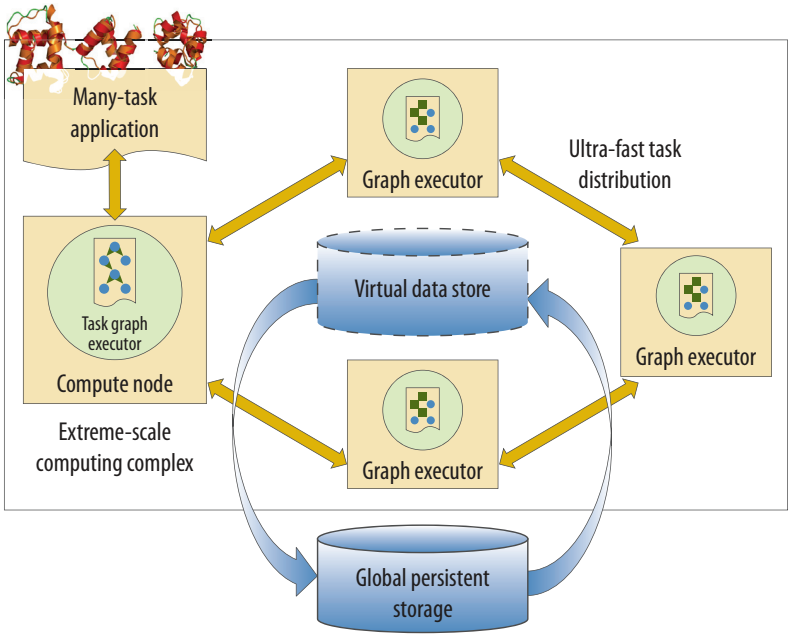
Hydrogen is the most abundant element in the universe. It is an environmentally friendly, clean fuel that has the potential to reduce the nation's dependence on foreign oil, improve the environment, and boost our economy. However, hydrogen fuel presents a safety challenge. The fuel is very energetic and prone to accidents. In certain conditions, a hydrogen-oxygen mixture can react violently and detonate. The process of transition from slow burning to a detonation is called a deflagration-to-detonation transition or DDT. Predicting DDT in various combustion settings remains an outstanding combustion theory problem. Led by Alexei Khokhlov with The University of Chicago, the High Speed Combustion and Detonation (HSCD) project uses ALCF resources to perform first-principles, reactive flow Navier-Stokes fluid dynamic simulations of DDT. These extremely detailed computer models allow researchers to safely study how hydrogen burns. Ultimately, this knowledge may help make hydrogen a viable fuel alternative for powering vehicles and other industrial applications.

Computer Science

ExM: System Support for Extreme-Scale, Many-Task Applications

Director's Discretionary Allocation: 3 Million Hours
PI: Michael Wilde (wilde@mcs.anl.gov) | Argonne National Laboratory

Exascale computers will enable and demand new problem-solving methods that involve many concurrent, interacting tasks. Running such "many-task" applications efficiently, reliably, and easily on extreme-scale computers is challenging. System software designed for today's mainstream, single program multiple data (SPMD) computations does not typically scale to the demands of many-task applications. Michael Wilde from Argonne National Laboratory is leading the ExM project to produce advances in computer science and

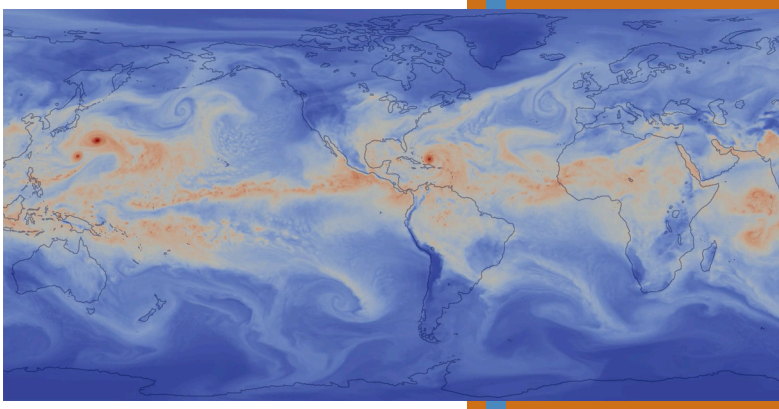


usable middleware that enable the efficient and reliable use of exascale computers for new classes of applications. The project is accelerating access to exascale computers for important existing applications and facilitating the broader use of large-scale parallel computing by new application communities for which it is currently out of reach. ExM project goals aim to achieve the technical advances required to execute many-task applications efficiently, reliably, and easily on petascale and exascale facilities. ExM researchers are developing middleware that will enable new problem solving methods and application classes on these extreme-scale systems. Researchers are evaluating ExM tools on three science applications—earthquake simulation, image processing, and protein/RNA interaction.

Earth Science

How Can More Intricate Climate Models Help Curb Global Warming?

INCITE Allocation: 40 Million Hours
PI: Warren Washington (wmw@ucar.edu) | National Center for Atmospheric Research (NCAR)

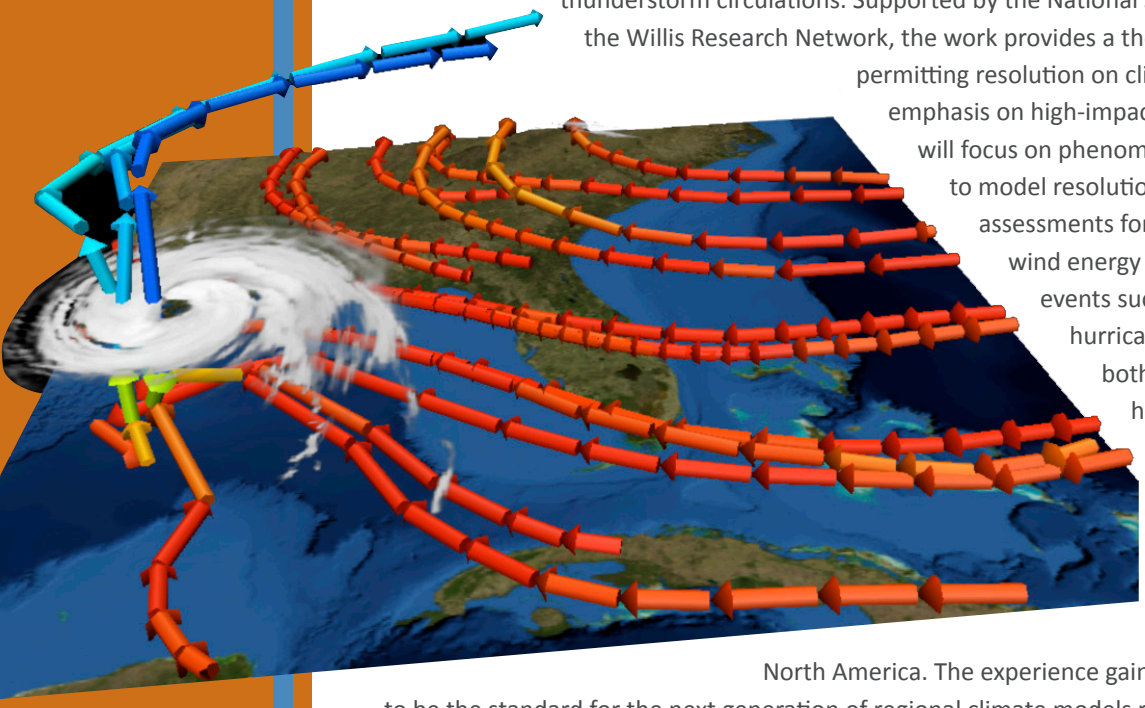


Global warming increases the occurrence of droughts, heat waves, wildfires, and floods. By improving the understanding of global warming's impact, society can optimally address climate adaptation considerations. Advanced computation allows researchers Warren Washington (NCAR), Mark Taylor (Sandia National Laboratories), Joe Insley and Robert Jacob (Argonne National Laboratory) and Andy Bauer (Kitware) to develop more complex and intricate climate models. The vital information these improved models provide will help guide environmental policy. Using ALCF resources, the Climate Science Computational End Station (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 method, called HOMME, is included in the CAM-SE model and has run with a resolution as high as ⅛th of a degree of latitude on more than 80,000 cores. Next, researchers will use CAM-SE to perform standard climate model benchmark simulations for comparisons with other models. They will also test new versions of the Community Earth System Model on the ALCF's Blue Gene/P.

Simulating Regional Climate at Convection-Permitting Resolution

Director's Discretionary Allocation: 13 Million Hours
PI: Greg Holland (gholland@ucar.edu) | National Center for Atmospheric Research

Researchers at the National Center for Atmospheric Research (NCAR) and the ALCF are using the Nested Regional Climate Model (NRCM) on the ALCF's Blue Gene/P to demonstrate the opportunities and challenges of simulating regional climate at sufficient resolution to resolve individual thunderstorm circulations. Supported by the National Science Foundation and the Willis Research Network, the work provides a thorough test of convection-permitting resolution on climate timescales with an emphasis on high-impact weather and climate. Analysis will focus on phenomena that have high sensitivity to model resolution, including water-snowpack assessments for the mid- and western U.S., wind energy assessments, and high-impact events such as winter storms and hurricanes. Researchers are simulating both the record-breaking 2005 hurricane season and winter storms of 2005/2006 on Intrepid, the ALCF Blue Gene/P system, using 4 km grid spacing for a region covering the entire North Atlantic Basin and most of North America. The experience gained at a resolution that is set to be the standard for the next generation of regional climate models represents an essential step towards the overarching goal to better quantify high-impact weather under climate variability and change. This will advance scientists' understanding of Earth's climate for national emergencies and broaden the community of researchers capable of using leadership computing resources.

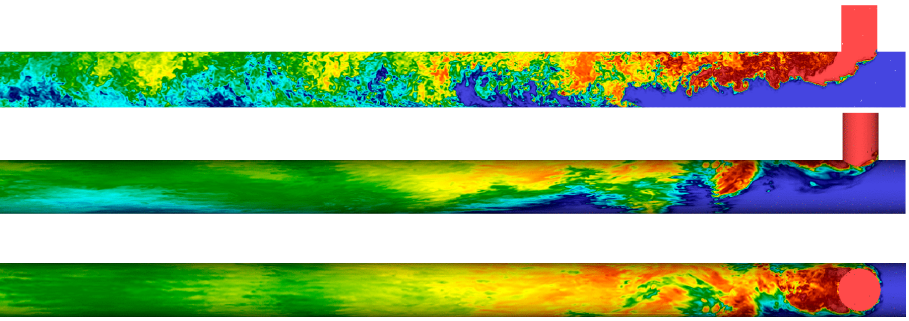


Energy Technologies

Advanced Reactor Thermal Hydraulic Modeling

INCITE Allocation: 25 Million Hours
PI: Paul Fischer (fischer@mcs.anl.gov) | Argonne National Laboratory

Advanced nuclear reactors are a key technology for providing power at a reasonable cost and with a low carbon footprint. This research is focused on analysis of thermal-hydraulics (heat transfer and coolant flow) in next-generation sodium- and gas-cooled nuclear reactors. The project simulations span a broad range of modeling scales. An important role for the compute-intensive simulations is to provide validation data for lower-cost reactor design simulations based on reduced-order models or subchannel codes.



During a worldwide validation effort for nuclear simulation codes, the Nuclear Energy Agency/ Organization for Economic Co-operation and Development (NEA/OECD) conducted a blind-benchmark study in 2010. Participants submitted computational results for velocity and temperature distributions in a T-junction (where streams of differing temperatures merge with limited mixing) that are important to understanding thermal-mechanical fatigue in light water reactors. Results were compared against experiments conducted for the benchmark. Staff worked with the project team from Argonne National Laboratory and Lawrence Berkeley National Laboratory to enable the Nek5000 code to scale up to 163,840 cores on Intrepid, the IBM Blue Gene/P (BG/P) system at the ALCF. This was leveraged in a workshop using the Juelich BG/P, where 19% of peak was realized on 262,000 cores. Runs from this project ranked first of 29 in temperature and sixth in velocity.

Large-Eddy Simulation for Green Energy and Propulsion Systems

INCITE Allocation: 20 Million Hours
PI: Umesh Paliath (paliath@ge.com) | GE Global Research

An understanding of the complex turbulent mixing noise sources for wind turbine airfoils and jet exhaust nozzles is critical to delivering the next generation of "green," low-noise wind turbines and jet engines. Scientists at GE Global Research are developing and proving hi-fidelity direct-from-first-principles predictions of noise to characterize these hard-to-measure acoustic sources. A scalable, compressible Large Eddy Simulation (LES)–based Computational Aeroacoustics (CAA) solver is being used to study free-shear layer noise from jet exhaust nozzles and boundary layer noise sources from airfoils. GE's LES strategy pushes application/validation to realistic conditions and scale, addresses fundamental physics and source characterization challenges, and extends capability to handle complex system interactions.

Powered by scalability improvements at the ALCF, earlier INCITE work demonstrated how this first-principles-based LES capability can transform product development. The research under way for jet engines will demonstrate (a) a numerical jet-noise rig that provides faster, cheaper, and additional details of the turbulent flow-fields than possible via physical experimentation, helping to explain how various chevron designs affect noise; and (b) the ability to capture propulsion-airframe integration effects such as the effect of pylon and jet-flap interaction. For wind turbines, simulations are in progress to demonstrate LES readiness in guiding low-noise design, validation of the complex scaling of turbulent self-noise, and the use of effective wall-models to enable large-span blade computations. The latter are needed to drive noise-reduction concepts beyond low-noise airfoil design.

Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air

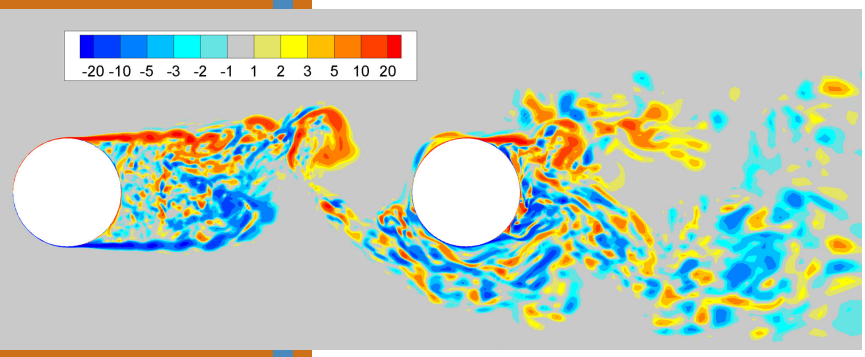
INCITE Allocation: 25 Million Hours
PI: Jack Wells (wellsjc@ornl.gov) | Oak Ridge National Laboratory

A rechargeable Lithium/Air battery can potentially store five to ten times the energy of a Lithium/Ion battery of the same weight, making practical widespread use of fully electric cars. But realizing this enormous potential is a very challenging scientific problem. Therefore, an interdisciplinary effort from IBM Research, Vanderbilt University, Oak Ridge National Laboratory (ORNL), and Argonne National Laboratory (ANL) is focusing on this problem. Currently, the main challenges are to realize a high percentage of the theoretical energy density, improve electrical efficiency of recharging, increase the number of times the battery can be cycled, and improve the power density. As the key reaction product in a Lithium/Air battery, various properties of Li_2O_2 remain elusive and needed to be explored. Thus, at Argonne, the current primary focus is on the basic study of lithium oxides (Li_2O), the peroxides (Li_2O_2) system (e.g., bulk crystals, surfaces, and nanoparticles) that resides on the cathode interfaces as the Li/Air cells' main reaction products. So far, the fundamental understanding of these systems that are governed by electronic, structural, and thermodynamic properties have been obtained by using the well-parallelized Density Functional code installed on Intrepid, the IBM Blue Gene/P system at the ALCF. These results will provide useful insights for the design of Li/Air cells in solving the discharge/recharge reactions at the electrode-electrolyte interface in the future.

Engineering

Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders

INCITE Allocation: 45 Million Hours
PI: Philippe Spalart (philippe.r.spalart@boeing.com) | Boeing

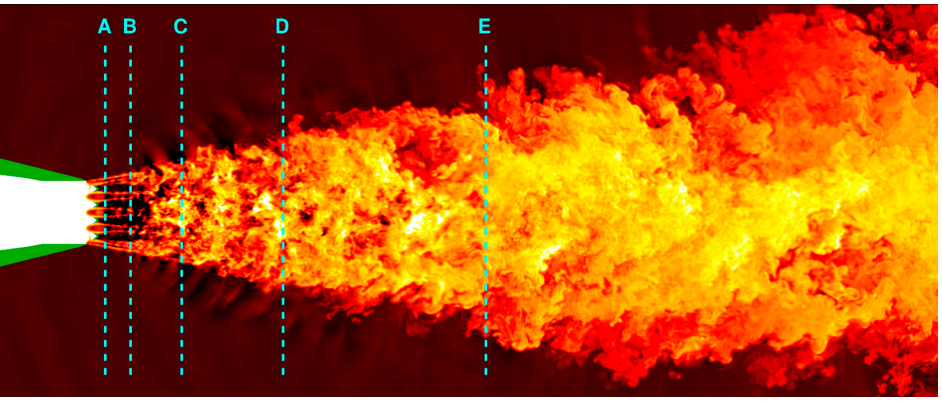


Researchers led by Dr. Philippe Spalart at Boeing are conducting a thorough numerical investigation of the turbulence and noise generated by Tandem Cylinders, a prime test case for detailed comparisons among computational fluid dynamics (CFD) and computational aero-acoustics (CAA) approaches, and with NASA experiments. It involves massive separation, the impingement of turbulence on a solid body, and the resulting noise. These features are typical in aircraft landing gear, wind turbines, bridges, heat exchangers, and buildings. The simulations reflect the state of the art in turbulence-resolving CFD approaches to massively separated flows. The IBM Blue Gene/P at the ALCF allows fine grids (up to 60 million cells) and wide domains (up to 16 cylinder diameters), with either periodic or free-slip boundary conditions in the lateral direction. The objective is to gain insight into the fundamental problem of low-Mach-number aero-acoustic computations. Very low Mach numbers are notorious for affecting CFD convergence; furthermore, the acoustic energy is minute. The accuracy of the simulations in the turbulent region is illustrated by the Power Spectral Density of velocity at a point in the wake: the inertial range of frequencies with exponent -5/3 is a decade long, revealing the turbulent energy cascade. The mean and unsteady wall pressures also compare well with experiments.

A central issue of aero-acoustics for low-Mach-number flows is the accuracy of noise predictions made using only the solid-surface terms in the Ffowcs-Williams-Hawkings (FWH) integral. It is widely assumed that this convenient simplification suggested by Curle is adequate for airframe noise. The researchers' work on a landing gear, however, failed to confirm this even at a Mach number as low as 0.115; this is also the case at Mach 0.1285, for the higher frequencies. This unexpected finding is being explored, including the effect of numerical resolution and dissipation, first inside the turbulence and then in the radiated noise, via the FWH equation. In addition, the researchers are computing the noise generated by so-called "long span bodies," extruded from a two-dimensional section. A series of simulations and FWH noise computations carried out with different spanwise sizes of the domain ranging from 1.5*D* up to 16*D* (the size of the model in the NASA experiments) confirmed the validity of the noise correction proposed, thus allowing a significant reduction of the span size of the computational domain in LES, and therefore, of the overall cost of the simulations.

Prediction of Supersonic Jet Noise Using Large-Eddy Simulation

ALCC Alloction: 60 Million Hours
PI: Parviz Moin (moin@stanford.edu) | Center for Turbulence Research, Stanford University



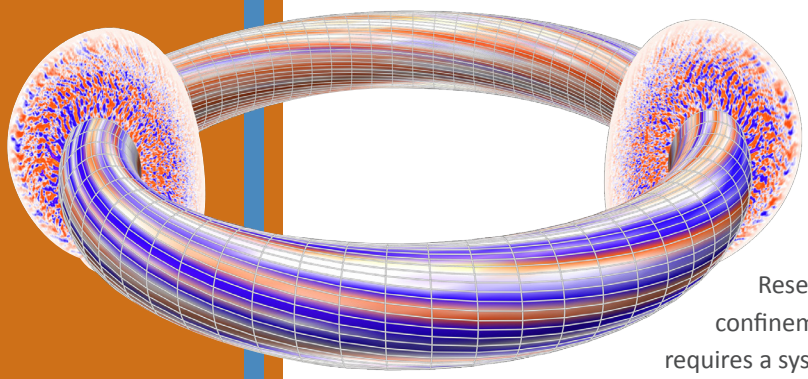
Noise generated by engine exhaust jets is one of the greatest barriers to the deployment of high-speed commercial aircraft. Very high jet velocities, typical of supersonic aircraft, heighten noise pollution levels in airport communities and accelerate hearing loss for crew on aircraft carrier decks. Modifying the nozzle geometry by adding chevrons (serrated geometric edges) to the nozzle lip is experimentally known to reduce jet noise, but the physical reasons for this are not well understood. Small-scale turbulence and shocks generated by chevrons strongly influence the development of the large turbulent eddies far downstream that control the production of noise. To capture these effects, compressible Large-Eddy Simulation using unstructured grids, which minimizes numerical dissipation and dispersion, is needed. For this purpose, the CharLES computational infrastructure, developed at the Center for Turbulence Research, is being used for these massively parallel simulations at the ALCF.

Using ALCF resources, researchers are working to fully resolve the effects of chevrons and heating on the noise produced in supersonic turbulent flow from a rectangular nozzle. For the first time, they are able to predict the far-field acoustic spectra from such a complex nozzle at all angles, including the broadband shock-associated noise. These simulations and comparisons with companion experiments are revealing new insight into how enhanced shear-layer mixing due to chevrons sustains itself and to address the question of the optimal chevron penetration angle from a jet-noise standpoint. Predictive, validated simulations such as these made possible by leadership computing facilities are critical to the design and viability of next-generation supersonic aircraft.

Fusion

Global Simulation of Plasma Microturbulence at the Petascale and Beyond

Early Science Program Allocation: 50 Million Hours
PI: William Tang (tang@pppl.gov) | Princeton Plasma Physics Laboratory



As scientists look for alternatives to fossil fuels to meet the world's energy needs, there is increasing interest in nuclear fusion, the power source of the sun. Of utmost importance in the design and operation of future fusion power sources is an understanding of turbulent transport losses. Acquiring this knowledge requires computational efforts at the extreme scale.

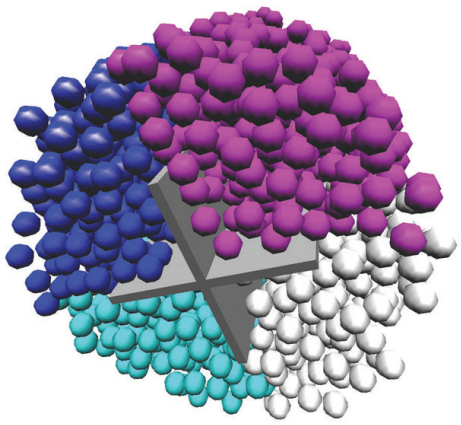
Researchers are studying the influence of plasma size on confinement properties in advanced tokamak systems, like ITER. This requires a systematic analysis of the underlying nonlinear turbulence characteristics in magnetically confined tokamak plasmas that span the range from current scale experiments, which exhibit an unfavorable scaling of confinement as the plasma radius increases, to ITER-scale plasmas, expected to be insensitive to size variations. Present-day tokamaks are not even one-third the radial dimension of ITER, making high-fidelity predictive simulations even more critical, since improvements in ITER-sized devices can only be validated after they are constructed and operational. In dealing with this challenge, researchers are deploying the GTC-P and GTS codes, which are highly scalable particle-in-cell gyrokinetic codes used for simulating microturbulence-driven transport in tokamaks. Efforts to scale the codes to the petascale power of the next-generation Blue Gene/Q have yielded significant results.

Materials Science

ALCF's Blue Gene/P Enables New Insights into Concrete's Flow Properties

INCITE Allocation: 25 Million Hours
PI: William George (william.george@nist.gov) | National Institute of Standards and Technology

Flow simulations of thousands of irregularly shaped particles on the ALCF's Blue Gene/P supercomputer are enabling new insights into how to measure and control flow properties of large-particle dense suspensions like concrete that can't be accurately measured in industrial settings. This study of the flow of matter—known as rheology—will provide a better understanding of concrete's flow properties to help ensure its optimum performance and eliminate cost overruns. Computing the flow allows researchers to correctly interpret empirical measurements in terms of fundamental units. Through their simulations

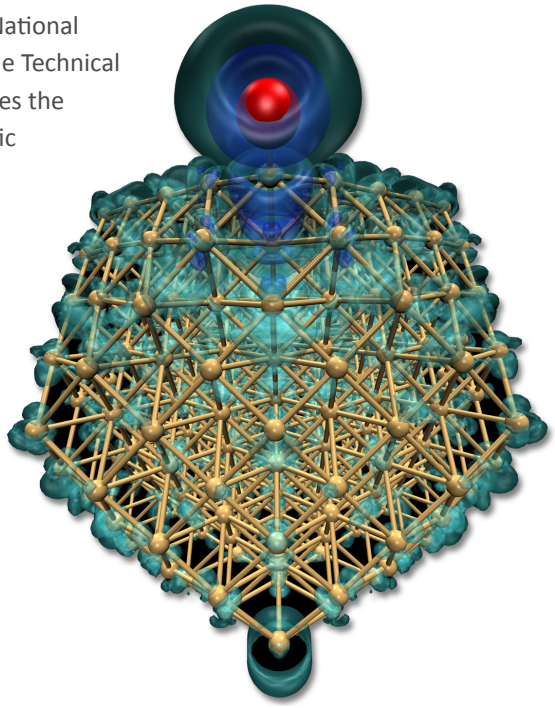


on the Blue Gene/P at the ALCF, researchers led by William George from the National Institute of Standards and Technology (NIST) have gained fundamental new insights into the yield stress of dense suspensions. Studies by the group indicate that particle contacts are an important factor in controlling the onset of flow in dense suspensions. Further, such interactions can be strongly influenced by the shape of the aggregates and lead to jamming effects that restrict the easy placement of concrete in forms. The researchers also discovered that for suspensions with a non-Newtonian fluid matrix, the local shear rates between aggregates strongly determine their rheological properties. These results have been validated against physical experiments with excellent agreement. Knowledge gained through this research has technological application in the building, coatings, water-treatment, food-processing, and pharmaceutical industries.

Better Catalytic System Designs through Nanoscale Research

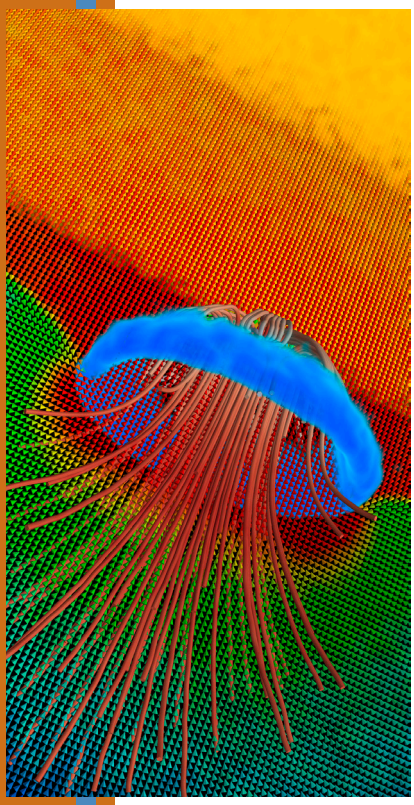
INCITE Allocation: 15 Million Hours
PI: Jeff Greeley (jgreeley@anl.gov) | Argonne National Laboratory

In life, sometimes to get the ball rolling, a little nudge is needed. In a chemical reaction, that nudge often comes in the form of a catalyst. A catalyst is an agent that speeds a chemical reaction along, or causes a reaction that otherwise would not have occurred. Platinum, a common catalyst, is used in catalytic converters to remove toxins from exhaust. Improved emissions control requires an understanding of how catalysts behave at their most fundamental atomic level—the nanoscale. Jeff Greeley at Argonne National Laboratory leads a team, including researchers from the Technical University of Denmark and Stanford University, that uses the supercomputing resources at the ALCF to study catalytic nanoparticles. Calculating catalysis on particles with as few as one thousand atoms takes several days on the world's fastest supercomputers. The process is so time intensive and the calculations are so complex, the research would be impossible without a leadership-class system like the ALCF's Blue Gene/P. With access to the world-class computing resources needed to explore the behavior of catalysts at the nanoscale, Greeley and his team are paving the way for improved catalytic system designs with wide-ranging industrial applications.



Reactive MD Simulation of Shock-Induced Cavitation Damage

INCITE Allocation: 45 Million Hours
PI: Priya Vashishta (priyav@usc.edu) | University of Southern California



Maintaining the soundness of nuclear reactors is a major concern for scientists, engineers, and the general public. Among many factors, "cavitation erosion" of cooling system components is a significant mechanism for long-term degradation in nuclear power plants. Cavitation occurs when a liquid experiences rapid change in pressure that creates low-pressure cavities within the liquid. These cavities, or cavitation bubbles, cause stress when they collapse and hit a solid surface, and therefore cause deterioration of the surfaces of materials. However, cavitation bubbles also provide benefits. Nanobubbles are used to prevent Stress Corrosion Cracking (SCC)—the biggest reason the lifetime of nuclear reactors is shortened. When nanobubbles form, they create low-pressure regions, but when they collapse near a solid surface, the result is the creation of high-pressure areas that relieve the tensile stresses that cause SCC in the material.

To get a molecular-level understanding of nanobubble collapse near a solid surface, Priya Vashishta and his colleagues, Rajiv Kalia and Aiichiro Nakano, at the University of Southern California (USC) are using Intrepid, the IBM Blue Gene/P system at the ALCF, to simulate and unravel the complex mechanochemistry problem. The 1-billion-atom simulation is feasible because it runs efficiently on 163,840 cores, the full system. The goal of this nanobubble collapse simulation is to understand molecular processes to improve both the safety and longevity of nuclear reactors. The efficiency with which these simulations run on Intrepid results from the USC group's successful work on Nickel-Sulfur stress corrosion cracking, using an Argonne Director's Discretionary allocation in 2010. The Department of Energy widely used the team's earlier findings in the Congressional budget, and SciDAC featured the research as the most important highlight in a decade. Currently, the nanobubble collapse simulations are being conducted using the INCITE allocation.

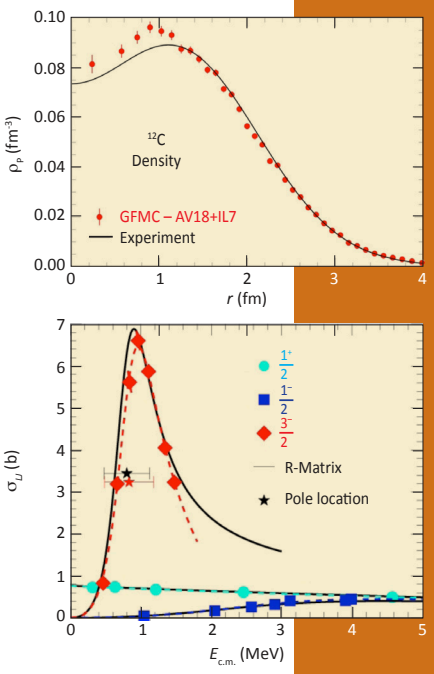
Nuclear Structure

Ab Initio Reaction Calculations for ^{12}C

Early Science Program Allocation: 110 Million Hours
PI: Steve Pieper (spieper@anl.gov) | Argonne National Laboratory

This project aims to calculate several fundamental properties of the ^{12}C nucleus: the imaginary-time response, the one-body density matrix, and transition matrix elements between isospin-0 and -1 states. Using Green's Function Monte Carlo (GFMC), these calculations will allow researchers to reliably compute neutrino-^{12}C scattering, quasi-elastic electron scattering, and the results of older reactions, such as (π,π') on ^{12}C.

Such properties are critical to a real understanding of the physics of nucleonic matter. Electron scattering experiments in the quasi-elastic regime, where the dominant process is knocking a single nucleon out of the nucleus, are under way for a range of nuclei. The separation into longitudinal and transverse response allows study of the propagation of charges and currents, respectively, in the nucleus. The nontrivial changes from studies of the nucleon and deuteron to larger nuclei require processes beyond one-nucleon knockout. Researchers will compute the transition density matrices on a two-dimensional grid of the magnitudes of the initial and final positions and will make a partial wave expansion of the angle between the two vectors. These matrices will be used as inputs for a variety of reaction calculations. To address Blue Gene/Q-related issues for GFMC, researchers changed the format for some matrices from dense to compressed, realizing a universal improvement on Blue Gene architecture. Currently running on a mid-plane of Blue Gene/Q, the code shows one of the highest per-node performance improvements from Blue Gene/P to Blue Gene/Q.



Physics

Advancing the Understanding of Nuclear Structure

INCITE Allocation: 15 Million Hours
PI: James Vary (jvary@iastate.edu) | Iowa State University

Researchers from Iowa State University, 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, as well as 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 ALCF and the Cray XT at Oak Ridge National Laboratory. The BG/P research team has completed ground-state C calculations—a key milestone. The ground state represents the best converged *ab initio* calculations of C ever.

Cosmic Structure Probes of the Dark Universe

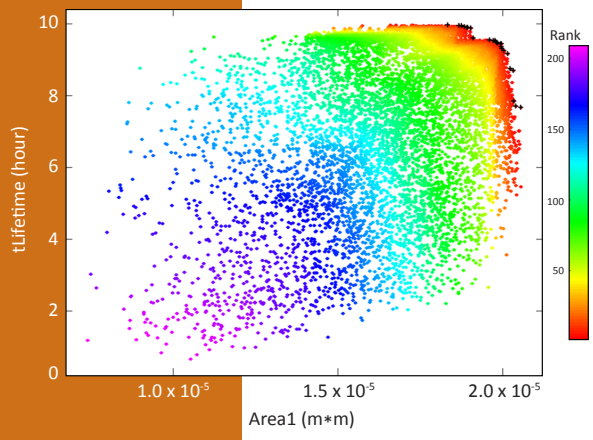
Early Science Program Allocation: 12 Million Hours
PI: Salman Habib (habib@lanl.gov) | Los Alamos National Laboratory

Dark energy and dark matter are the dominant components of the Universe. Their ultimate nature, however, remains a mystery. A team of researchers led by Salman Habib at Los Alamos National Laboratory is using the ALCF to carry out some of the largest high-resolution simulations of the distribution of matter in the Universe, resolving galaxy-scale mass concentrations over observational volumes representative of state-of-the-art sky surveys. A key aspect of the project will be a major simulation suite covering approximately a hundred different cosmologies — an essential resource for interpreting next-generation observations. This effort targets an approximately two- to three-orders-of-magnitude improvement over currently available resources. The database created from this project will be an essential component of Dark Universe science for years to come.

The simulation program is based around the new HACC (Hardware/Hybrid Accelerated Cosmology Code) framework aimed at exploiting emerging supercomputer architectures such as the IBM BG/Q arriving at Argonne in 2012. HACC's medium-resolution infrastructure has been tested for scalability on the current BG/P across the full machine and is now running on a BG/Q prototype system. Porting the high-resolution modules is currently in progress; the scaling properties of HACC do not depend on the short-range force calculations.

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

ALCC Allocation: 36 Million Hours
PI: Michael Borland (Borland@aps.anl.gov) | Argonne National Laboratory



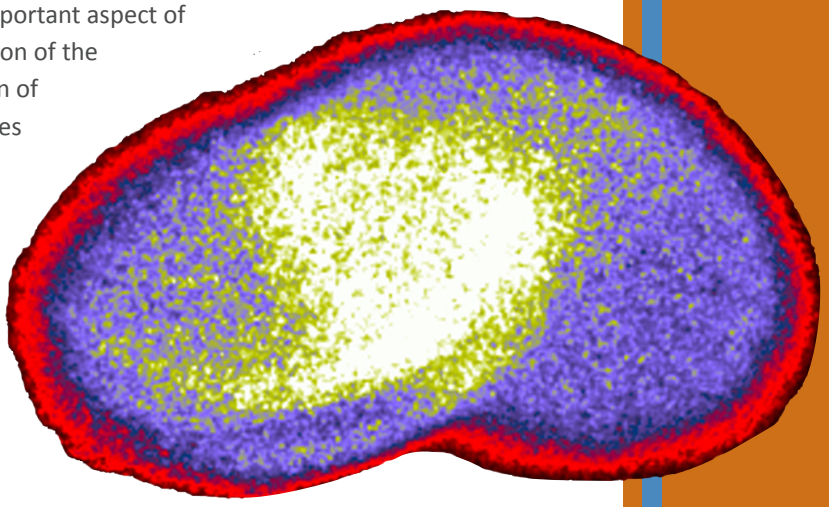
The brightest storage ring-generated x-ray beams in the Western Hemisphere are created by Argonne's Advanced Photon Source (APS) and are used by more than 5,000 scientists worldwide. A planned upgrade to the APS will reconfigure the facility's magnets (its "lattice") to enhance this world-class resource. The addition of long superconducting devices will increase brightness by an order of magnitude for x-rays above 20 keV compared to standard APS devices. 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.

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 Blue Gene/P at the ALCF with the APS-developed code "elegant" to create complex particle-tracking simulations. Researchers will use a portion of their ALCC allocation to advance important concept work for next-generation "ultimate" storage rings.

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

INCITE Allocation: 50 Million hours
PI: Denise Hinkel (hinkel1@llnl.gov) | Lawrence Livermore National Laboratory

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. 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 allocated to Intrepid, the Blue Gene/P system at the ALCF.

ALCF Resources for Breakthrough Science

The ALCF's major computing resources include the IBM Blue Gene/P systems Intrepid, Challenger, and Surveyor. Intrepid has a peak speed of 557 Teraflops (TF) and is dedicated to production science. Challenger has a peak performance of 13.9 TF and is used to debug and develop. Surveyor is a nearly 14-TF, single-rack system used for tool and application porting, software testing and optimization, and systems software development. Soon to come: Mira, a powerful 10-petaflops IBM Blue Gene/Q system, will run programs at 10 quadrillion calculations per second.

Intrepid

Named Intrepid, this Blue Gene/P system has a highly scalable torus network, as well as a high-performance collective network that minimizes the bottleneck common in simulations on large, parallel computers.

Blue Gene applications use common languages and standards-based MPI communications tools.

Intrepid consists of

- 40 racks;
- 1,024 nodes per rack;
- 40,960 quad-core compute nodes (163,840 processors);
- 640 I/O nodes;
- 88 GB/s, 7.6PB storage;
- 80 TB of RAM.

Challenger

Challenger is the home for the prod-devel job submission queue. It is intended for small, short, interactive debugging and test runs. Challenger has 1,024 quad-core nodes (4,096 processors) and two terabytes of memory. Peak performance is 13.9 TF.

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

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 has

- 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

Intrepid connects to other research institutions using a total of 20 GBs of public network connectivity. This allows scientists to transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and the Metropolitan Research and Education Network (MREN).

Mira

Mira, IBM's next-generation Blue Gene/Q supercomputer, will be delivered to the Argonne Leadership Computing Facility (ALCF) in 2012. Computational scientists and engineers look to the speed, memory size, and disk storage capacity of this leadership-class system to propel innovation in science and technology. The 10-petaflops supercomputer will feature 48K 16-way compute nodes (768K processors), and 768 terabytes of memory. Like the ALCF's Intrepid, an IBM Blue Gene/P system, Mira will be made available to scientists from industry, academia, and government research facilities around the world.

Tukey

Being installed in 2012, Tukey will be twice as fast as its predecessor, Eureka. It will be based on NVIDIA Fermi GPUs with double precision floating points, which will make it a powerful, general-purpose analysis and computation engine. The 200 GPUs are rated at an aggregate 103 teraflops in double precision. Tukey will share the Mira network and parallel filesystem, enabling direct access to data generated by Mira simulations.

2011 ALCF PUBLICATIONS

Researchers who use Argonne Leadership Computing Facility (ALCF) resources are major contributors to numerous publications that document their breakthrough science and engineering. The refereed journal articles and conference proceedings represent research ventures undertaken at the ALCF through programs supported by the U.S. Department of Energy and Argonne National Laboratory. These documented efforts are tangible evidence of the ALCF's major contribution to key advances in a wide range of scientific disciplines, including astrophysics, biological sciences, chemistry, computer science and mathematics, earth sciences, engineering, materials science, nuclear physics, and plasma physics.

This list contains 132 publications in descending order of their publication dates. To view their abstracts, visit the ALCF website (http://www.alcf.anl.gov/publications).

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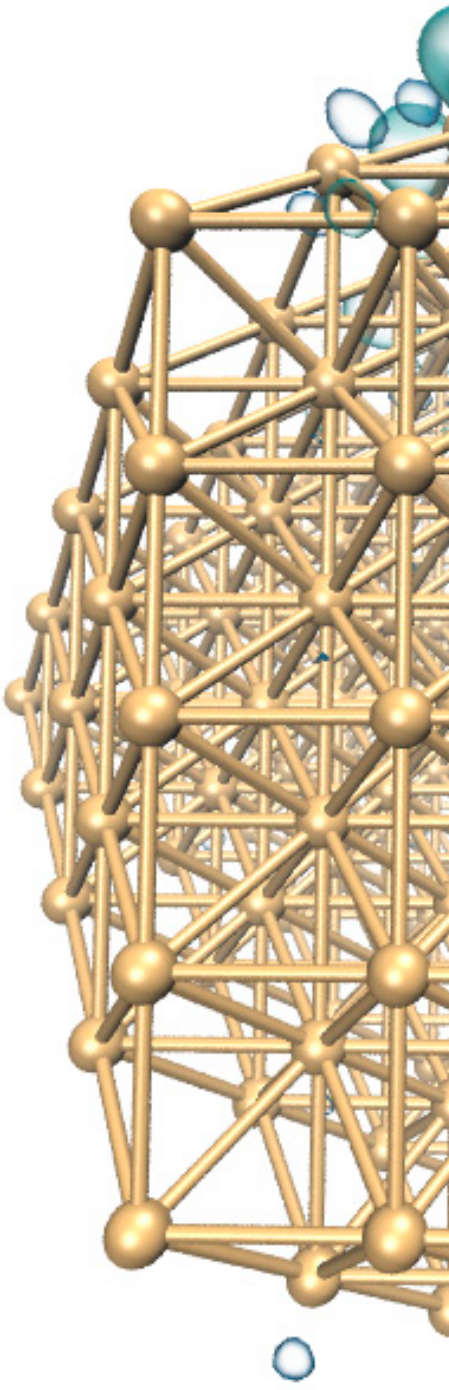

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