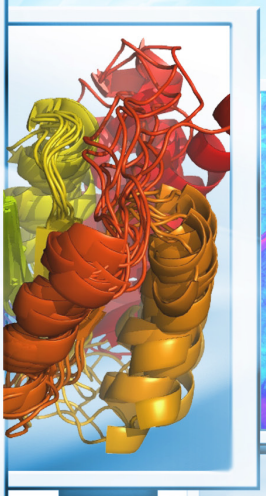
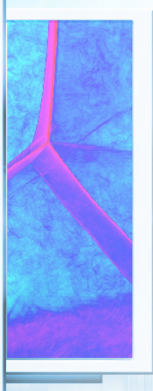
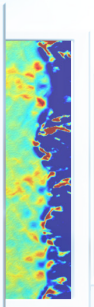
Argonne Leadership Computing Facility

Inspiring Innovation in Industry through Science







Staying competitive and innovative in your industry may require advanced computing capability that is too complex or costly to maintain in-house. At the Argonne Leadership Computing Facility (ALCF), you can easily tap into high-performance computing systems to tackle key science and engineering challenges. Whether you need resources for small-scale modeling and simulation or large-scale, computationally intensive projects, the ALCF can meet a wide range of near- and long-term computational needs.

The ALCF houses Intrepid, an IBM Blue Gene/P, one of the world's fastest computers for open science. Intrepid enables users to address a wide array of problems in science and engineering at unprecedented scale and speed. Despite its power, the energy-efficient system uses one-third the electricity of comparably sized machines built with more conventional parts. President Obama awarded IBM with a National Medal of Technology and Innovation for its Blue Gene family of supercomputers.

Using ALCF resources, industry collaborators are making breakthrough discoveries that will enable:

- Unprecedented reductions in emissions and noise in aircraft engines and wind turbines,
- Improved consumer products through a better understanding of how suds form and break down,
- Insights on mechanisms controlling the flow and spread of concrete to help solve quality control and material properties problems.

www.alcf.anl.gov

Argonne NATIONAL LABORATORY

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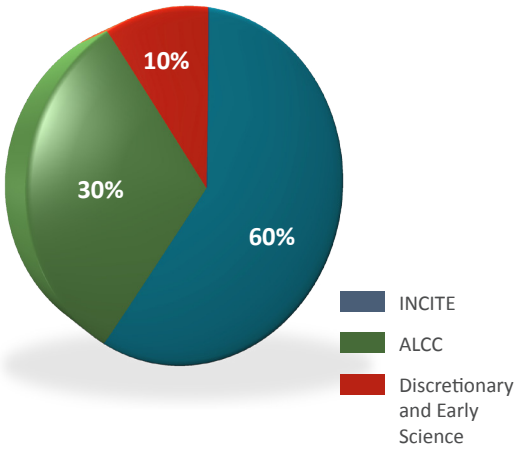
"The ALCF welcomes users from industry. Our dedicated team of computational scientists, performance engineers, systems administrators, and technical support specialists work with corporations both large and small to enable breakthrough science and engineering. We encourage your application for ALCF resources through one of our allocation programs. Time and assistance for open research is provided at no cost, while access for proprietary research is charged on a cost-recovery basis. No matter the type of research, ALCF stands ready to help you reach the next level in analysis, simulation, and visualization."

David Martin
ALCF Manager of User Services and Outreach

World Class Computational Center

One of two premier U.S. Department of Energy (DOE) leadership-class computing facilities, the ALCF aims 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.



Research is conducted at the ALCF using computer time awarded through four major programs:

- Innovative and Novel Computational Impact on Theory and Experiment (INCITE),
- ASCR Leadership Computing Challenge (ALCC),
- Early Science,
- Director's Discretionary.

(For program details, see www.alcf.anl.gov)

Blue Gene/P Resources at the ALCF

Industry researchers typically receive access to Intrepid, a 557-teraFLOPS Blue Gene/P supercomputer. The ALCF also provides 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. A test and development system for visualization is open to users as well.

In 2012, an even more powerful system will be available to ALCF users—Mira, a 10-petaFLOPS IBM Blue Gene/Q system. This supercomputer will be 20 times faster than the Blue Gene/P, running programs at 10 quadrillion calculations a second. Argonne 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 currently have been beyond reach, not just due to their sheer size, but because of their inherent uncertainties and unpredictability.

ALCF Resources

Intrepid

Production scientific and engineering computing

- 40,960 quad-core compute nodes (163,840 processors)
- Memory: 80 TB
- 6.5 PB disk storage
- Peak Performance: 557 TF

Eureka

Converts data output to visual representations

- 100 dual quad-core servers
- 200 Quadro FX5600 GPUs in the S4s
- Memory: 3.2 TB+ RAM
- Peak Performance: More than 111 TF

Data Storage

Blue Gene/P data systems

- 640 I/O nodes
- 16 storage area networks (SANS)
- 7,680 disk drives
- 7.6 PB raw storage
- 88 GB/second transfer speed
- 2 parallel file systems—PVFS and GPFS

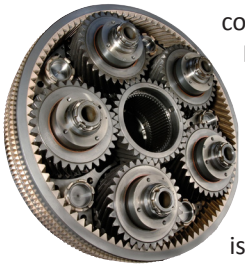
Networking

Internally, Intrepid uses five different networks. The main one is a 3D torus with an aggregate bandwidth of 5.1 Gbps to each node. Connectivity to outside institutions is provided by 20 Gbps of bandwidth to commercial and research networks.

ALCF/Industry Collaborations

Some of the world's most well-known and highly regarded companies have sought Argonne's computing capability and technical expertise to convert that knowledge into transformative products and technologies for industry. Among them are Pratt & Whitney and Procter & Gamble. Others who have used ALCF resources to benefit their industry applications include General Electric Global Research and the National Institute of Standards and Technology.

Improving Aircraft Engine Combustor Simulations

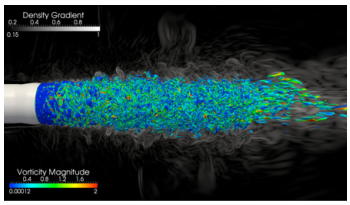


Pratt & Whitney (P&W) explored leading-edge combustor design methods using DOE INCITE allocations on the Blue Gene/P. The research led to improved capabilities and reduced solution times for three-dimensional combustor simulations. It has enabled the depth of understanding needed to meet emissions goals. P&W is applying these improvements to the company's next-generation engine to deliver unprecedented reductions in emissions, noise, and cost of ownership as compared to current engines.

"In an ever-expanding global economy where technology leadership is critical to competitiveness, INCITE provides American industry with an engine for technological and competitive growth."

—Pete Bradley, Pratt & Whitney

Delivering "Green," Low-Noise Wind Turbines and Jet Engines

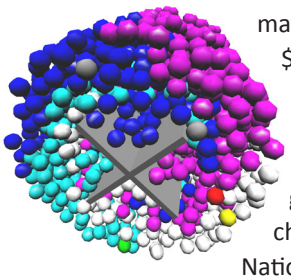


Understanding the complex turbulent mixing noise sources for wind turbine airfoils and jet exhaust nozzles is vital to delivering the next generation of "green," low-noise wind turbines and jet engines. Using ALCF resources, scientists at GE Global Research are investigating methods to reduce airfoil trailing edge noise—a key component in wind turbine noise generation. Predicting noise from first principles, while numerically expensive, is a promising method to characterize noise for hard-to-measure details and sources.

"Simulation-based aeroacoustics via large-scale computing—the focus of this collaboration with ALCF—is a key enabler to tackling the yield-limiting noise barrier for wind turbines."

—Dr. Gary Leonard, GE Global Research

Gaining New Insights into the Flow Properties of Concrete

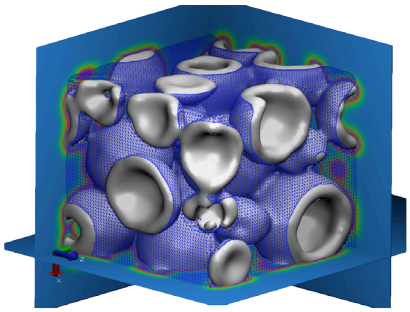


Concrete is the most widely used building material in the world, representing a $100 billion industry in the United States that is crucial for the nation's physical infrastructure. Modeling the flow of concrete represents a great scientific and computational challenge. Researchers from the National Institute of Standards and Technology are leveraging the computational resources of the Blue Gene/P to shed light on the mechanisms that control the flow and spread of concrete. A successful outcome of this research will help solve critical outstanding problems in the cement and concrete industry in regards to quality control and assessment of fresh concrete properties as new source materials and novel mix designs are developed. Insight from these studies has technological application in the building, coatings, water-treatment, food-processing, and pharmaceutical industries.

"Realistic simulations of dense suspensions like concrete demand significant computational resources in order to produce results with predictive capability."

—William George, National Institute of Standards and Technology

Developing Better Consumer Products



Procter & Gamble (P&G) researchers used the Blue Gene/P system at the ALCF to investigate the molecular mechanisms of bubble formation in foams. Their DOE INCITE allocation allowed them to perform computer simulations at an unprecedented scale on the dissolving of soap and foaming of suds. An understanding of how suds form and break down is critical in the development of many consumer goods, foods, and fire control materials. Ultimately, the work is expected to help P&G formulate products faster and more efficiently. The consumer wins by getting better products sooner, and at better value, than would have been possible using traditional methods.

"We wouldn't be able to conduct a computational experiment of this size without our partnership with Argonne. Through this research, we have experienced a dramatically exciting new approach to evaluate materials."

—Tom Lange, Procter & Gamble

Expert Consulting, Hands-on Help Available

ALCF experts in computational methods and application tuning provide in-depth assistance in using Intrepid, optimizing applications, and improving computational methods. They arm your researchers with technical details about Intrepid's architecture, give hands-on help in scaling and tuning applications on the supercomputer, and assist users with their visualization and analysis needs.

To maximize your time, ALCF staff delivers full project lifecycle assistance, value-added services, and support in conjunction with ALCF hardware and software resources. The ALCF can tailor services to meet the unique requirements of your research initiative and affords ongoing contact with knowledgeable ALCF computational scientists and performance engineers.

Furthermore, staff members help you port, tune, and parallelize your applications on Intrepid. They also address I/O and data analytics issues that inhibit performance.

Working in tandem with experts from Argonne's Mathematics and Computer Science Division, the staff provides extensive knowledge and experience in:

- Computer architectures;
- Computational algorithms;
- Porting, performance tuning, and parallelizing of scientific applications and other software;
- I/O; and
- Visualization.

For More Information

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To learn more about the ways that Argonne works with industry, visit www.anl.gov/techtransfer

Other Argonne User Facilities

Located near Chicago, Argonne National Laboratory is a multi-disciplinary research center with more than 200 research projects and roughly 3,200 employees from nearly 60 nations. It is one of the U.S. Department of Energy's oldest and largest laboratories. Argonne's mission is to apply a unique mix of world-class science, engineering and user facilities to deliver innovative research and technologies.

Besides the ALCF, Argonne's national scientific user facilities include the Advanced Photon Source, Center for Nanoscale Materials, and Transportation Research and Analysis Computing Center to benefit researchers from industry, academia, and government laboratories. As is the case with the ALCF, operating time in the facilities is available without charge to those who plan to publish their results in open literature. Proprietary research is accommodated on a full cost-recovery basis. For details about each facility, visit the Argonne website (www.anl.gov/Science_and_Technology).

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