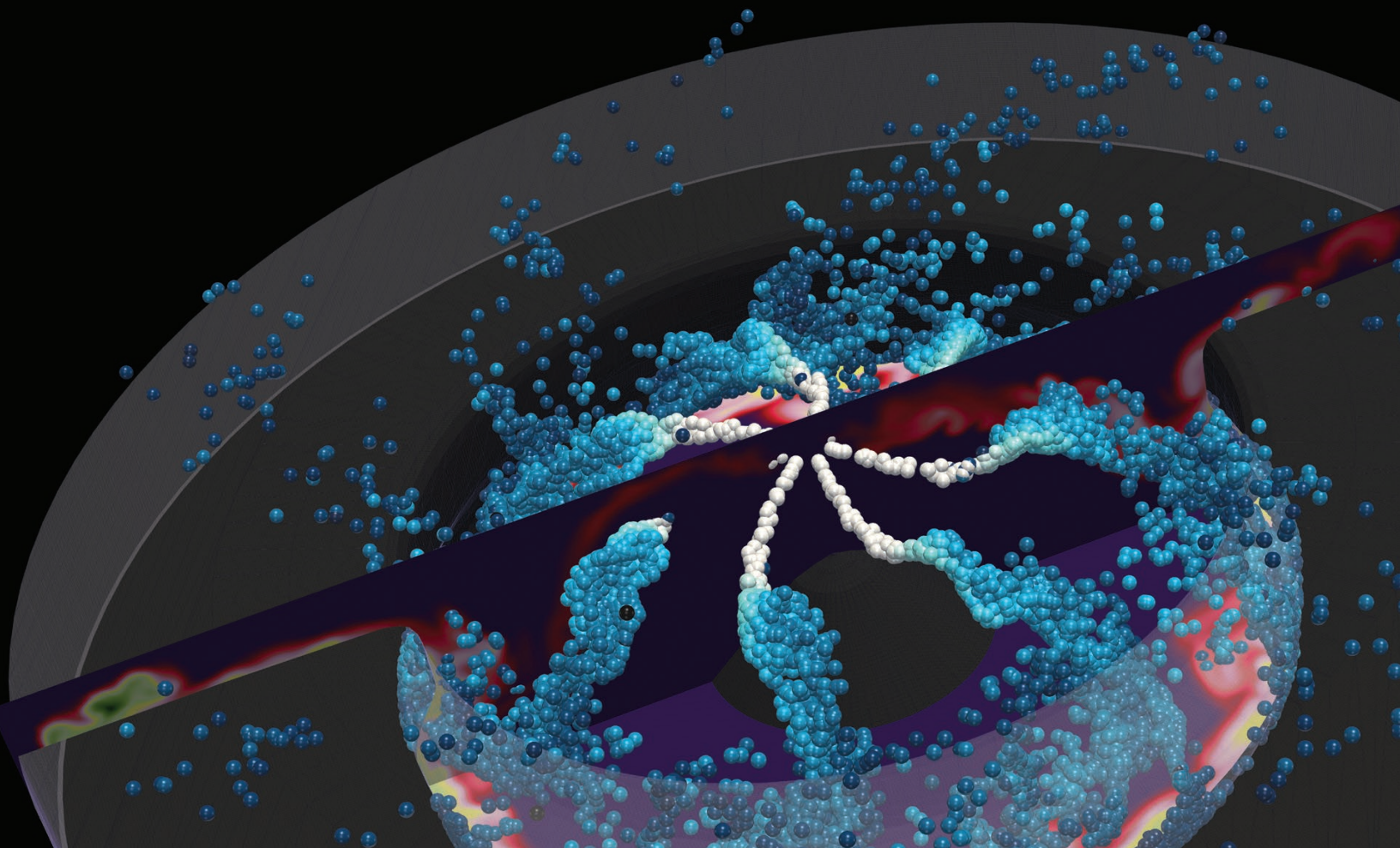
Argonne NATIONAL LABORATORY

2016 ANNUAL REPORT

ARGONNE LEADERSHIP COMPUTING FACILITY



On the cover: This simulation captures fuel distribution inside the combustion chamber of a GM 1.9 L diesel engine being operated in an advanced low-temperature combustion mode. High-fidelity 3D simulations provide unique insights into the fuel-air mixing process, which has enabled Argonne engineers to develop this combustion mode. The simulation was carried out on Mira, the ALCF's IBM Blue Gene/Q supercomputer, using the computational fluid dynamics software CONVERGE.

Image credit: Joseph A. Insley, Janardhan Kodavasal, and Sibendu Som, Argonne National Laboratory

ARGONNE LEADERSHIP COMPUTING FACILITY

ANNUAL REPORT 2016

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THE YEAR IN REVIEW

The Argonne Leadership Computing Facility (ALCF) helps researchers solve some of the world's largest and most complex problems, while also advancing the nation's efforts to develop future exascale computing systems. This report presents some of the ALCF's notable achievements in key strategic areas over the past year.

DIRECTOR'S MESSAGE

The year 2016 marked the ALCF's 10th year in existence — a major milestone for a premier high-performance computing facility whose computing resources have pushed boundaries in science and engineering in ways and at speeds once believed impossible.

In the span of a single decade, we have deployed a succession of supercomputers that have gone from the terascale to petascale. We've helped modernize and optimize key community codes used across a wide range of disciplines. We've forged partnerships to help U.S. companies stay competitive. And we have 10 years of experience serving a scientific community with an insatiable appetite for what's next and what's possible.

It's a good a time to reflect on how far we've come as an organization, and how much we've accomplished.

Each new system the ALCF rolls out represents the state of the art in computing power and capabilities. This continued evolution is allowing researchers to tackle increasingly complex problems, gain insights more quickly, and perform more precise simulations of everything from combustion engines to the human brain.

The recent arrival of our newest system, Theta, has given us a glimpse of the future of leadership computing. Project teams from the Theta Early Science Program, the first researchers to gain access to the new system, are already reporting notable performance gains. Meanwhile, our primary production supercomputer, Mira, continues to serve as a reliable and powerful tool for many scientific achievements, including the development of a new coating material to reduce friction and the design of novel peptides to advance tailored drug design.

This year we also kicked off the ALCF Data Science Program, a pioneering initiative aimed at preparing data-centric applications for leadership computing resources. Forward-looking efforts like the ADSP, and others, are helping our nation maintain its leadership role in advancing scientific discovery through high-performance computing.

As we look ahead to another exciting year in 2017, I would like to thank our staff, our users, and our collaborators for making the ALCF what it is today. And while we have seen breakthrough after breakthrough in the past decade, the next decade will be an even more exciting time for science and technology.

Michael E. Papka
Division Director, ALCF;
Deputy Associate Laboratory Director,
Computing, Environment, and Life Sciences

ABOUT ALCF

The Argonne Leadership Computing Facility provides supercomputing capabilities to the scientific and engineering community to advance fundamental discovery and understanding in a broad range of disciplines.

Supported by the U.S. Department of Energy's (DOE) Office of Science, Advanced Scientific Computing Research (ASCR) program, the ALCF is one of two DOE Leadership Computing Facilities in the nation dedicated to open science.

Available to researchers from universities, industry, and government agencies, the ALCF is a DOE Office of Science User Facility that helps accelerate the pace of discovery and innovation by providing supercomputing resources that are 10 to 100 times more powerful than systems typically used for scientific research.

Through substantial awards of supercomputing time and user support services, the ALCF enables large-scale modeling and simulation research aimed at solving some of the world's largest and most complex problems in science and engineering.

2016 STATS

6.6+
BILLION CORE-HOURS OF TOTAL COMPUTE TIME

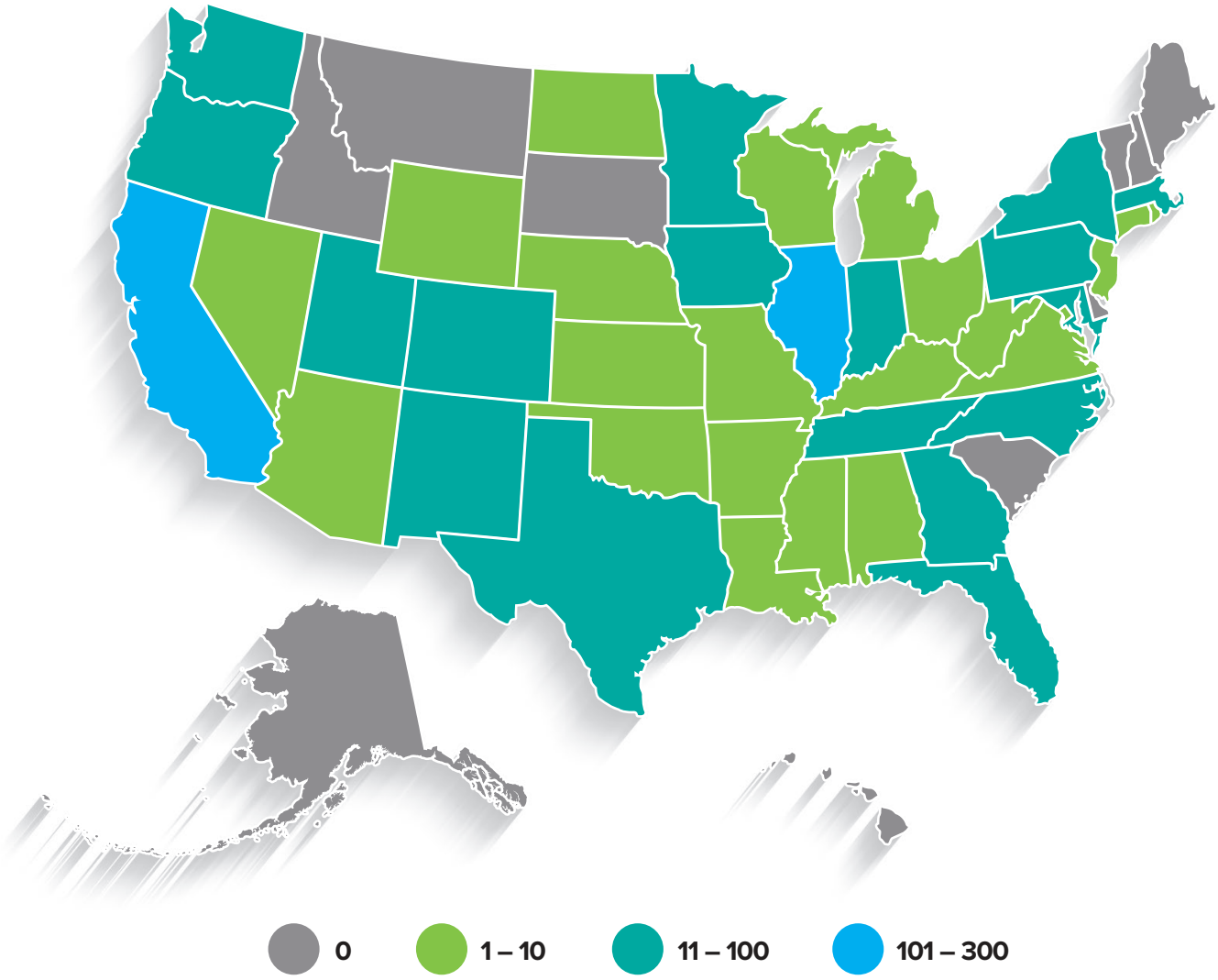
300+
ACTIVE PROJECTS*

1,000+
FACILITY USERS*

250+
PUBLICATIONS

*FISCAL YEAR 2016

2016 ALCF USERS BY STATE



2016 ALCF USERS BY AFFILIATION

ALCF LEADERSHIP

OPERATIONS

Mark Fahey

DIRECTOR OF OPERATIONS

Advanced Integration, HPC Infrastructure, HPC Storage, HPC Systems & Network Administration

SCIENCE

Katherine Riley

DIRECTOR OF SCIENCE

Computational Science, Data Sciences, Performance Engineering, Visualization & Data Analysis

USER EXPERIENCE

Richard Coffey

DIRECTOR OF USER EXPERIENCE

Business Intelligence, Communications, Industrial Outreach, Technical Support

ALCF teams play a critical role in supporting the facility's supercomputing environments, the user community, and their efforts to accelerate scientific discoveries.

OPERATIONS

Mira had another excellent year in 2016, exceeding all key metrics for availability and utilization. Our new system, Theta, was delivered and installed this summer. Thanks to the dedication and expertise of our acceptance team, who worked closely with staff from Intel and Cray to debug and address technical issues, Theta was accepted six months ahead of schedule. We also successfully ported our Cobalt scheduler to Theta so it was ready to run jobs as soon as the system was released to Early Science Program users.

We made several upgrades to our storage capabilities in 2016. To improve our archival capacity, we installed a third eight-frame tape library with approximately 24 petabytes using LTO6 media. We deployed the GPFS/HPSS Interface (GHI) file migration tool on one of our scratch filesystems, and will soon deploy it on the other filesystem. Members of our team also developed and launched Bloodhound, a system-monitoring tool that performs wellness checks on our storage systems and provides continuous alerts on critical hardware and software changes. Additionally, we launched sbank, a new allocation accounting system that provides users with more flexibility in querying project usage data.

In the coming year, we will bring Theta into full production mode, while continuing to prepare for the arrival of Aurora. We also expect to deploy our burst buffer-like storage cache, and new data transfer nodes and data movers for the archives.

– Mark Fahey

SCIENCE

While Theta's arrival generated some new excitement in 2016, it was Mira that continued enabling our user community to pursue science and engineering breakthroughs. In 2016, ALCF project teams produced more than 250 research publications, including papers in high-impact journals such as *Science*, *Nature*, and *Physical Review Letters*. Theta did get some use as well, as researchers from our Early Science Program achieved notable performance gains and scaling results while preparing for their science campaigns. Next year, we'll be kicking off the Early Science Program for Aurora, and continuing our close collaboration with Intel and Cray to prepare applications and our user community for the facility's next-generation supercomputers.

In our rapidly evolving community, it's critical that we operate with an eye on the future. This year, we were involved in some key efforts aimed at helping the nation move closer to realizing a future exascale system, including DOE's Exascale Requirements Reviews and the Exascale Computing Project (ECP). For the ECP effort several members of our team will continue to be deeply engaged in projects to develop applications and software for exascale machines. In addition, we launched the ALCF Data Science Program, as well as a new data science team, to explore and improve the computational tools and techniques needed to enable future data-driven discoveries on leadership computing resources.

– Katherine Riley

USER EXPERIENCE

The User Experience team is responsible for making sure ALCF users have a positive and productive experience with our facility, our services, and our supercomputers. Our goal is to help to reduce friction, remove roadblocks, and support the needs and goals of the scientists and engineers who use our leadership computing resources.

Stewarding the large-scale projects that are awarded computing time at the ALCF requires a significant amount of communication and assistance to the principal investigators and their teams. By using best practices and continuous improvement techniques, we ensured project teams were on-boarded quickly and efficiently so they could begin their science campaigns as soon as their allocations began. We also helped bring our users' stories to life by communicating the impact of their work to the scientific and HPC communities, our sponsors, and the general public.

On the outreach side, we connected the ALCF to a variety of new industry users, extended our user training offerings, and hosted the annual meeting of the Intel® Xeon Phi™ User's Group. We've also been making significant strides with business intelligence. Not only have we improved the efficiency of the ALCF's data management and analysis activities by centralizing all of the facility's critical data, we have ensured our internal and external reports are as accurate as possible.

– Richard Coffey

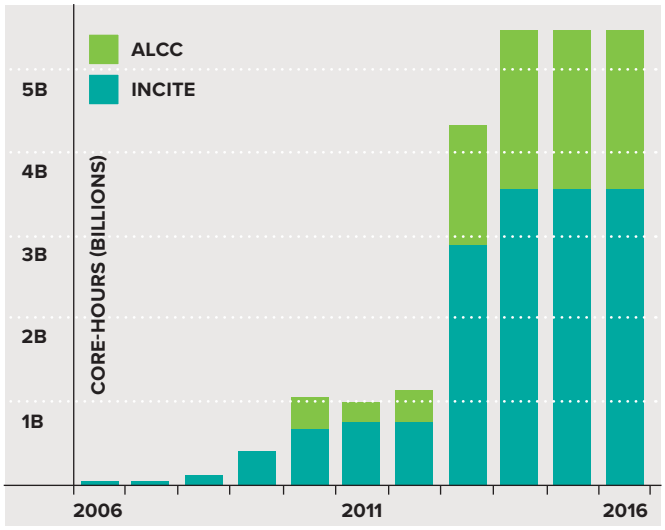
10-YEAR ANNIVERSARY

A DECADE OF GROWTH AND IMPACT

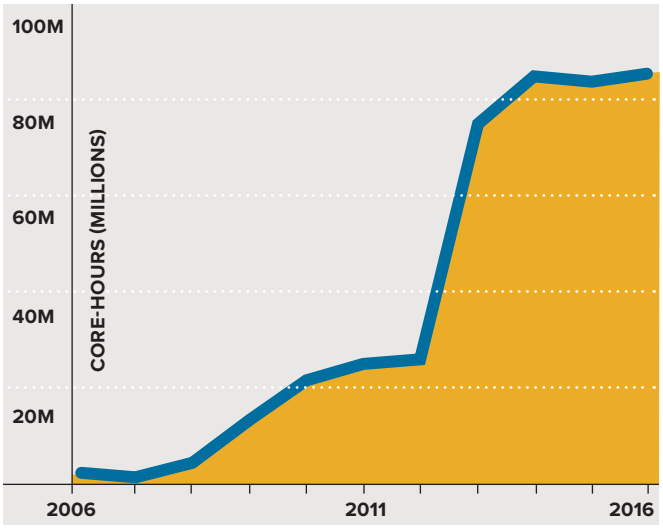
In its first decade of existence, the ALCF has played a significant role in advancing discovery and innovation through high-performance computing.

The ALCF was established at Argonne National Laboratory in 2006 as part of a DOE initiative dedicated to enabling transformational advances in science and engineering by providing the most powerful supercomputers in the world for open scientific research. The facility has grown leaps and bounds in its first decade, developing and deploying leading-edge computing systems with unprecedented capabilities, while fostering an ever-growing user community that is pushing the boundaries of fundamental discovery and understanding in a broad range of scientific disciplines.

TOTAL ALLOCATED HOURS



AVERAGE PROJECT SIZE



The ALCF's two primary allocation programs – INCITE and ALCC – have grown along with the facility. With each new supercomputer, these programs have awarded increasingly larger allocations of computing time to researchers.

THE HISTORY OF ALCF SUPERCOMPUTERS

IBM Blue Gene/L
2005–2008

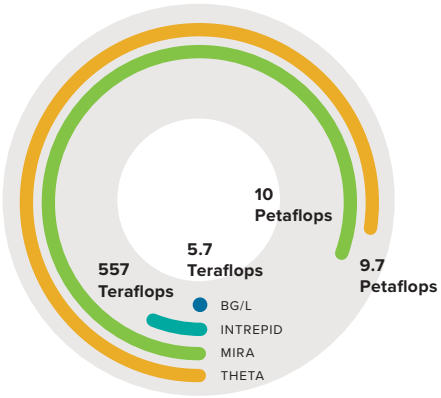
Intrepid, IBM Blue Gene/P
2008–2013

Mira, IBM Blue Gene/Q
2012–

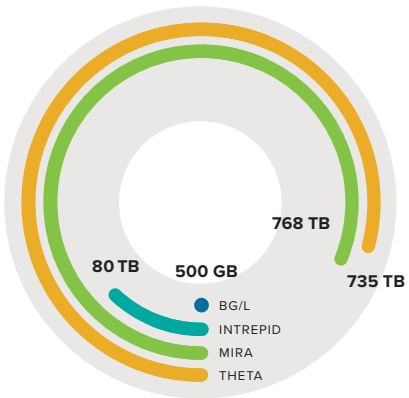
Theta,
Cray/Intel® Xeon Phi™
2016–

From teraflops to petaflops, ALCF supercomputers have come a long way over the past decade. Each new system brings advanced capabilities that enable researchers to expand their investigations in both scale and scope.

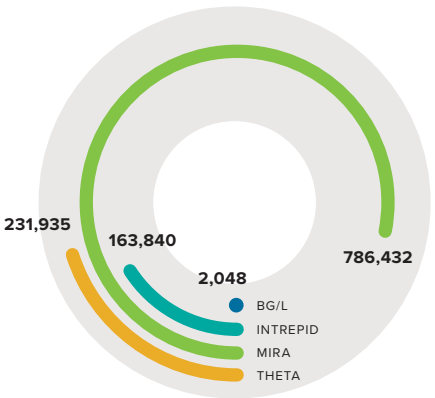
ALCF SYSTEM SPECS



PEAK PERFORMANCE



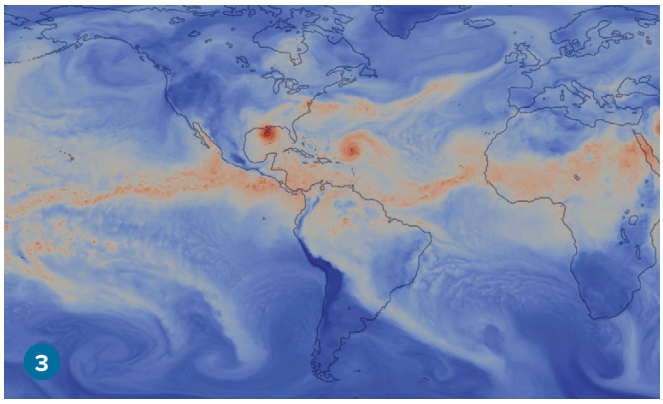
MEMORY



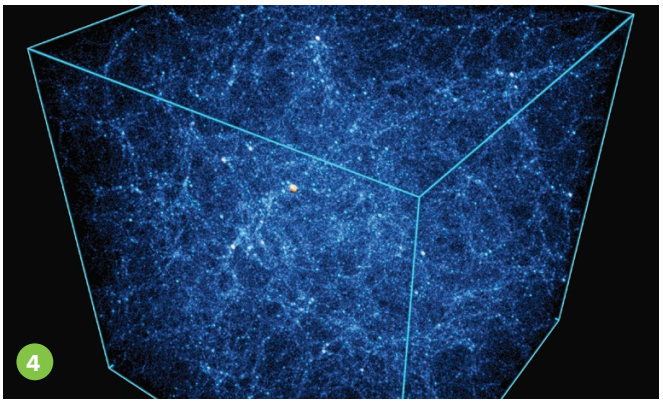
CORES

10-YEAR ANNIVERSARY

To acknowledge a decade of breakthrough science, here is a look at some notable accomplishments made possible by the ALCF's computing resources and expertise.



A snapshot from the Community Atmosphere Model. Image credit: Joseph A. Insley, Robert Jacob, and Sheri Mickelson, Argonne National Laboratory; Andy Bauer, Kitware; Mark Taylor, Sandia National Laboratories



This visualization shows the distribution of matter in the Outer Rim simulation. Image credit: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory

ENERGY TECHNOLOGIES

1. Adding Renewables to the Electric Grid

Mihai Anitescu
Argonne National Laboratory

Adding renewable energy to the electric grid is tricky, because solar and wind generation fluctuate with weather conditions. A team of researchers used ALCF resources to demonstrate that a complex mathematical approach called stochastic optimization can help grid operators minimize instability and distribute power on demand while minimizing the need for costly backup plants.

MATERIALS SCIENCE

2. Developing New Types of Concrete

William George
National Institute of Standards and Technology

Concrete is essential to modern life, but its production releases a significant amount of greenhouse gases. To develop new formulas that reduce emissions, scientists modeled the flow of concrete and found new principles that should help guide the design of more environmentally friendly types of concrete.

EARTH SCIENCE

3. Enhancing Climate Predictions

Warren Washington
National Center for Atmospheric Research

When we want to know how the climate might change in the future — which areas might have more drought, more floods, more heat — we turn to climate models. But predicting the future on a global climate scale is extraordinarily difficult; it's so complex that slight changes to the parameters show different futures. The ALCF has been helping scientists run these enormous climate models and refine the techniques to provide more accurate simulations.

PHYSICS

4. Illuminating the Early Universe

Salman Habib
Argonne National Laboratory

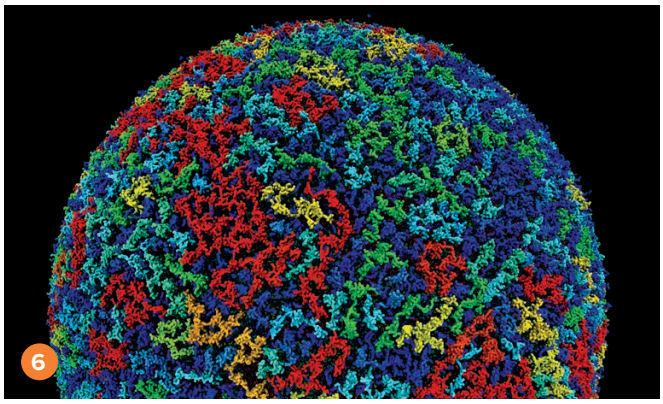
The Outer Rim simulation, one of the largest cosmological simulations ever run, modeled the evolution of the universe over billions of years, allowing scientists to "watch" as galaxies develop. This helps researchers understand how cosmic structures are formed and provides a new tool for studying the mysterious force called dark energy.

ENGINEERING

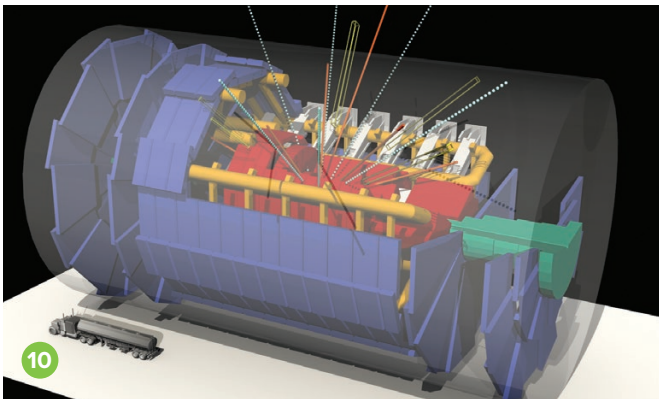
5. Improving Airplane Engines

Peter Bradley
Pratt & Whitney

Inside a jet engine, air flowing faster than a hurricane is combined with fuel to generate heat that powers the plane. Designers are turning to supercomputers to model these complex processes to make new engines that are cleaner, quieter, and less expensive. A study at the ALCF was key to helping industry integrate supercomputer simulations into their design process. Improvements based on this work are now currently in use in aircrafts.



Nanocarbon produced by oxidation of a silicon-carbide nanoparticle. Image credit: Joseph A. Insley, Argonne National Laboratory; Ken-ichi Nomura, University of Southern California



An artist's representation of particle collisions in the ATLAS detector at CERN's Large Hadron Collider. Image credit: Taylor Childers, Joseph A. Insley, and Thomas LeCompte, Argonne National Laboratory

MATERIALS SCIENCE

6. Investigating How Materials Crack

Priya Vashishta and Rajiv Kalia
University of Southern California

When materials crack and corrode under stress, the process starts at the molecular level. Only supercomputers have the capability to run simulations so detailed that they actually show how molecules propagate a crack over time. These simulations can help researchers design possible solutions, such as self-healing nanomaterials, to build safer, stronger materials for high-stress environments.

CHEMISTRY

7. Modeling Detonations to Transport Explosives Safely

Martin Berzins
The University of Utah

Using ALCF supercomputers, researchers modeled an explosion that left a 30-by-70-foot crater in a Utah highway, capturing the physics that made the truck's cargo explode more violently than it should have. With such simulations, engineers can design safer transport for explosives.

BIOLOGICAL SCIENCES

8. Puzzling Out Proteins that Work Against Antibiotics

T. Andrew Binkowski
Argonne National Laboratory

In the race against antibiotic resistance, computing is becoming a valuable tool for identifying new ways to fight disease. Researchers ran simulations on key pathogen proteins, including nine molecules that could work against anthrax. They also explored potential avenues to defeat a gene that confers resistance against even the strongest antibiotics.

BIOLOGICAL SCIENCES

9. Understanding the Molecular Basis of Parkinson's Disease

Igor Tsigelny
University of California, San Diego

Researchers ran simulations to understand how several proteins connected with Parkinson's disease interact to cause the degenerative neurological disorder. The findings provide a test bed for identifying possible treatments via computer modeling.

PHYSICS

10. Using Supercomputers to Analyze Particle Collisions

Thomas LeCompte
Argonne National Laboratory

At the Large Hadron Collider (LHC) in Europe, the most powerful accelerator in the world, physicists run simulations on the data collected from particle collisions in order to understand the fundamental forces that drive the universe. To explore the potential of supercomputers to enable future discoveries at LHC, a research team adapted their code to run on ALCF computing resources, allowing them to analyze more data and simulate more complex events than previously possible.

SHAPING THE FUTURE

ALCF researchers lead and participate in several strategic activities that aim to push the boundaries of what's possible in computational science and engineering.

ALCF Director Michael E. Papka addresses participants at the 2016 Intel® Xeon Phi™ User's Group annual meeting.


ALCF 2014-2015 SCIENCE HIGHLIGHTS

SHAPING THE FUTURE

ALCF'S NEXT-GENERATION SUPERCOMPUTERS

The ALCF hits major milestones with the acceptance of Theta and preparations for Aurora.

In 2016, the ALCF made significant strides toward its next-generation Intel-Cray systems with the successful delivery of Theta and the continued development of Aurora.

Aurora, a 200-petaflops system scheduled for delivery in 2018, will replace Mira as the ALCF's next major production supercomputer. Theta is designed to be a bridge between Mira and Aurora, providing an early Intel-Cray system that will enable new science while helping users transition their applications to the new technology.

Developed in collaboration with industry leaders Intel and Cray, Aurora and Theta are funded under DOE's Collaboration of Oak Ridge, Argonne, and Lawrence Livermore (CORAL) initiative, a joint procurement activity launched in 2014 to build state-of-the-art supercomputers that are essential for technology advancement and scientific discovery. The new ALCF systems will help ensure continued U.S. leadership in high-end computing for scientific research, while also cementing the nation's position as a global leader in the development of next-generation exascale computing systems.

Among the most notable milestones in 2016 was the successful installation and acceptance of Theta. The system was delivered to Argonne two months ahead of schedule, arriving at the ALCF in late June. Once the system was installed, ALCF staff members, in collaboration with Intel and Cray, worked diligently to integrate and evaluate the machine to prepare it for acceptance testing. The team's work included developing tests and tools to identify, debug, and resolve several technical challenges along the way. ALCF staff members were also instrumental in setting up and running many of the acceptance test codes while working with the vendors to analyze performance and correctness results.

A rendering of the ALCF's future 200-petaflops supercomputer, Aurora.

The collaborative efforts resulted in Theta being accepted on September 30, 2016, six months earlier than the initial target date for acceptance. Theta was subsequently made available to research teams in the Theta Early Science Program, and will be opened up to the broader ALCF user community in 2017.

On the Aurora front, the ALCF-Intel-Cray team made progress with the project's non-recurring engineering (NRE) work, which encompasses activities to enhance the usability and effectiveness of the final system. Much of the work in 2016 focused on facility infrastructure enhancements to prepare for the new supercomputer, including the installation of additional cooling capacity at Argonne's chilled water plant, an upgrade to Argonne's power station to accommodate Aurora's power requirements, and the completion of design plans for Aurora's electrical and cooling systems at Argonne's Theory and Computing Sciences Building, where the system will be installed. In addition, ALCF staff continues to work closely with the vendors to enhance the system's architecture, packaging, and software stack.

In July 2016, the ALCF issued a Call for Proposals for its Aurora Early Science Program, with the selected projects to be announced in early 2017. The program will award computing time to 10 science teams to pursue innovative research as part of pre-production testing on the new system. The projects will prepare key applications for the architecture and scale of Aurora and solidify libraries and infrastructure to pave the way for other applications to run on the system. To develop and optimize their applications for Aurora, project teams will be given access to early hardware, receive training on the underlying Intel and Cray technologies, and work collaboratively with ALCF staff and vendor experts.

"With the development of Theta and Aurora, we were able to continue evolving the many-core, homogenous architectures that our user community has grown accustomed to. These leading-edge systems will fuel a new era of scientific discoveries at the ALCF."
— Susan Coghlan, project director for Theta and Aurora

SHAPING THE FUTURE

THETA: PAVING THE WAY TO AURORA

Theta, the ALCF's new 9.65 petaflops supercomputer, will help bridge the gap between Mira and Aurora.

Designed in collaboration with Intel and Cray, Theta provides advanced capabilities that will enable breakthrough computational science and engineering research at the ALCF. The early production system will also help ALCF users transition their applications to the new Intel-Cray architecture.

Theta is designed to serve as a stepping stone to the ALCF's next leadership-class supercomputer, Aurora. Like Theta, Aurora will be a massively parallel, many-core system powered by Intel® Xeon Phi™ processors, running Cray's HPC software stack.

Theta is equipped with 3,624 nodes, each containing a 64-core processor with 16 gigabytes (GB) of high-bandwidth in-package memory (MCDRAM), 192 GB of DDR4 RAM, and a 128 GB SSD. Theta's initial parallel file system is 10 petabytes.

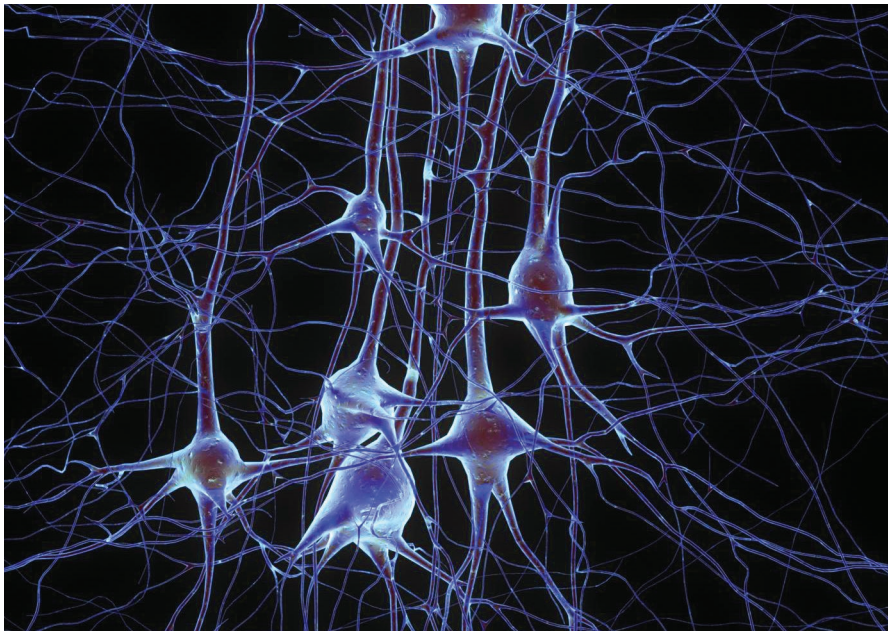
While Theta's peak speed is slightly less than Mira's, the new system has several features that will allow scientific codes to achieve higher performance. These features include:

- High-bandwidth MCDRAM (300-450 GB/s depending on memory and cluster mode), with many applications running entirely in MCDRAM or using it effectively with dynamic RAM (DRAM)
- Improved single-thread performance
- Potentially much better vectorization with AVX 512
- Large total memory per node (208 GB on Theta vs. 16 GB on Mira)

Theta is located in the machine room in Argonne's Theory and Computing Sciences Building.

THETA EARLY SCIENCE PROJECTS

The ALCF's Theta Early Science Program allocates preproduction time on the system to projects pursuing science and code development work.



Digital reconstruction of pyramidal cells. Image credit: Blue Brain Project, EPFL

Direct Numerical Simulations of Flame Propagation in Hydrogen-Oxygen Mixtures in Closed Vessels
Alexei Khokhlov, The University of Chicago
Code: HSCD

Free Energy Landscapes of Membrane Transport Proteins
Benoît Roux, The University of Chicago/Argonne National Laboratory
Code: NAMD

Next-Generation Cosmology Simulations with HACC: Challenges from Baryons
Katrin Heitmann, Argonne National Laboratory
Code: HACC

First-Principles Simulations of Functional Materials for Energy Conversion
Giulia Galli, The University of Chicago/Argonne National Laboratory
Codes: Qbox, WEST

Large-Scale Simulation of Brain Tissue
Fabien Delalondre, Blue Brain Project, EPFL
Code: CoreNeuron

Scale-Resolving Simulations of Wind Turbines with SU2
Juan J. Alonso, Stanford University
Code: SU2

CODE DEVELOPMENT PROJECTS

Advanced Electronic Structure Methods for Heterogeneous Catalysis and Separation of Heavy Metals
Mark Gordon, Iowa State University
Code: GAMESS

Electronic Structure-Based Discovery of Hybrid Photovoltaic Materials on Next-Generation HPC Platforms
Volker Blum, Duke University
Codes: FHI-aims, GAtor

Extreme-Scale Unstructured Adaptive CFD: From Multiphase Flow to Aerodynamic Flow Control
Kenneth E. Jansen, University of Colorado Boulder
Code: PHASTA

Flow, Mixing, and Combustion of Transient Turbulent Gaseous Jets in Confined Cylindrical Geometries
Christos Frouzakis, Swiss Federal Institute of Technology Zurich
Code: Nek5000

The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon
Paul Mackenzie, Fermilab
Codes: MILC, CPS

Quantum Monte Carlo Calculations in Nuclear Theory
Steven Pieper, Argonne National Laboratory
Code: GFMC

SHAPING THE FUTURE

EARLY SCIENCE TEAMS PREPARE THETA FOR SCIENCE ON DAY ONE

The ALCF's Theta Early Science Program (ESP) is designed to prepare users for the new supercomputer, ensuring that projects and codes are ready to make good scientific use of the system.

Researchers participating in the Theta ESP are getting the first crack at using the new supercomputer for science simulations. In the process, they are helping pave the way for other applications to run on the system.

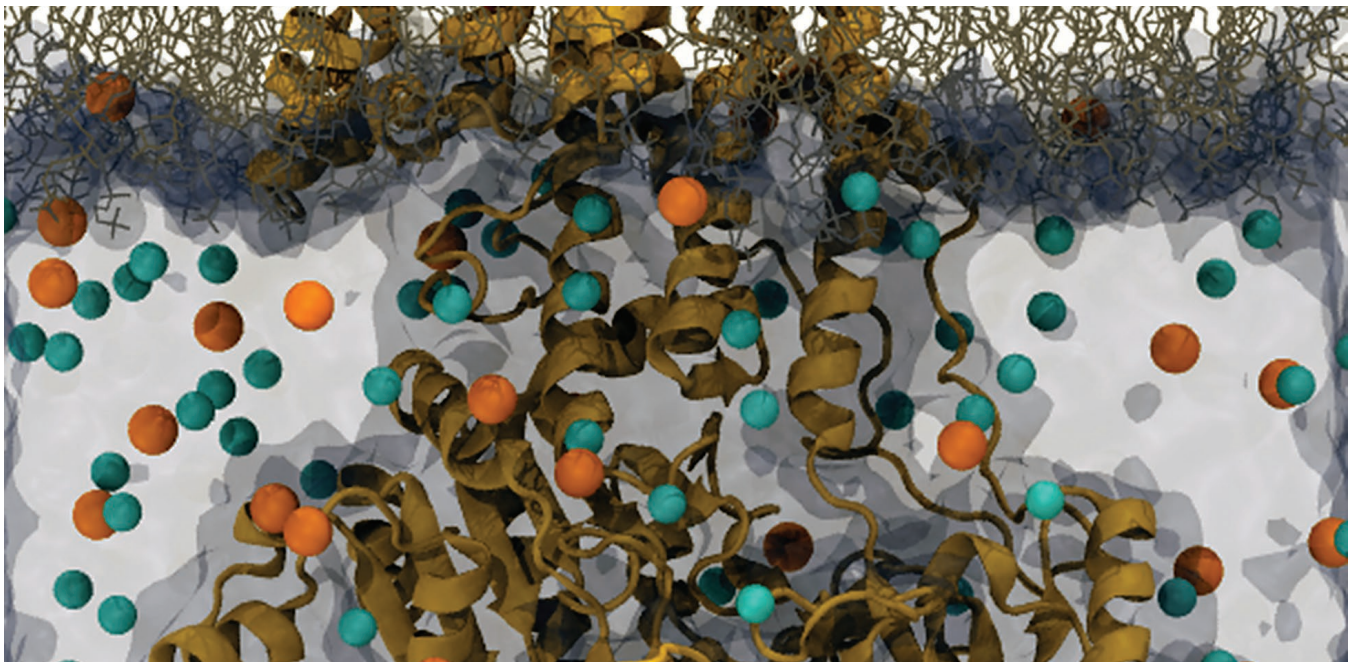
By bringing together computational scientists, code developers, and computing hardware experts, the program creates a collaborative environment for optimizing applications and characterizing the behavior of new hardware and software features.

Long before Theta was installed at Argonne this summer, ESP research teams, in collaboration with ALCF and vendor staff, were working diligently to adapt their applications for the system's new Intel-Cray architecture. Access to advanced Theta simulator software and early hardware allowed the teams to test and debug applications in advance of the system being available. The researchers were also able to use Mira and other ALCF computing resources for early development work that did not require Theta hardware (e.g., new algorithms, new physics modules).

In August, the ALCF hosted a hands-on workshop that allowed the ESP teams to use the full Theta system to port, benchmark, and optimize their applications. Attendees were able to measure the scaling of their applications on problem sizes relevant to their proposed science runs. They also received instruction on Intel and Cray development environments, system software, the Cobalt job scheduler, vendor development tools, and other essential information for running on Theta. In addition, the hands-on collaborative sessions allowed teams to try out different code optimization approaches and experiment with the system's innovative memory hierarchy. Many projects were able to scale up to 2,000–3,000 nodes on Theta, with some taking advantage of the full system. Project team members presented many of these benchmarks, as well as other performance measurements, at the 2016 Intel® Xeon Phi™ User's Group meeting held at Argonne in September.

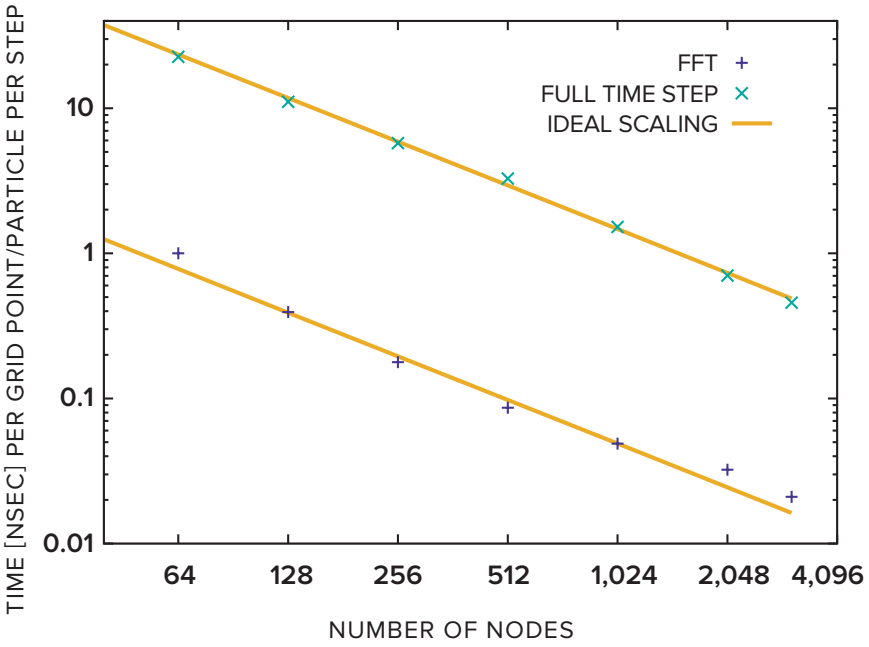
Now that Theta is operational, ESP teams have begun running science simulations on the system to pursue their research goals, which range from modeling the brain to simulating the evolution of the universe. When the Early Science period is completed, each team will produce a technical report detailing their efforts to port and optimize their codes for Theta. They will present their results and lessons learned at a wrap-up workshop open to the entire ALCF user community.

Researchers from the Theta ESP visited at ALCF for a hands-on workshop devoted to helping them port, benchmark, and optimize their applications on Theta.



Benoît Roux's ESP project aims to determine the free energy landscapes of large membrane proteins, especially P-type ATPases such as the sodium-potassium pump (shown in yellow). Image credit: Brian Radak, Argonne National Laboratory/The University of Chicago; Huan Rui, The University of Chicago

STRONG SCALING ON THETA



HACC strong scaling results on Theta for the entire application (indicated by teal "x" symbols), and for just the fast Fourier transform (FFT) part of the application (indicated by purple pluses). The solid lines show ideal scaling. The tests were carried out on up to 3,072 nodes.

EARLY RETURNS

While the Early Science period does not hit full swing until 2017, several research teams have already achieved notable scaling and performance improvements on Theta.

- In initial results for the GFMC code, researchers demonstrated strong OpenMP thread scaling on a node, with the best throughput achieved using several MPI ranks with fewer threads each. Weak scaling was excellent up to 3,168 nodes.
- The HACC team found their application performed remarkably well in a strong scaling test, evolving $2{,}048^3$ particles in an $(800\ h^{-1}\ Mpc)^3$ volume (the target size for their hydrodynamics simulations in the Early Science period).
- In NAMD scaling tests using up to 3,072 nodes on Theta, researchers observed a 10x speedup per node compared to the code's performance on Mira.
- For the Nek5000 code, researchers conducted a strong scaling test using a turbulent channel flow simulation. The code performed 7.2x faster per node compared to its performance on Mira.
- Researchers performed a strong scaling study with PHASTA on an 80-billion element mesh. The case scaled perfectly to 192,000 cores on Theta, and fit into the system's MCDRAM with 1.2 million elements per core.

SHAPING THE FUTURE

BEYOND AURORA: THE PUSH TOWARD EXASCALE

The ALCF is a key contributor to the DOE's Exascale Computing Project, a multi-laboratory initiative aimed at accelerating the development of a capable exascale computing ecosystem.

ECP Director Paul Messina provides an overview of the project at an Argonne town hall meeting.

In addition to developing and operating some of today's most powerful computing systems, the ALCF is actively involved in the pursuit of future exascale systems, which will deliver approximately 50 times more performance than the top supercomputers currently in use.

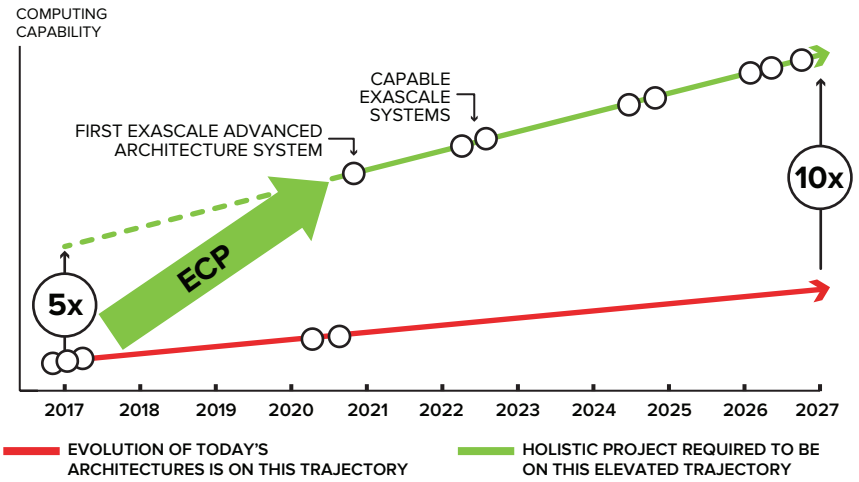
From identifying the science capabilities needed from extreme-scale supercomputers to exploring and pioneering the technologies that will power them, the ALCF has long been a key player in the nation's efforts to develop a future exascale computing system.

In 2016, the DOE announced the launch of the Exascale Computing Project (ECP), a collaborative effort of two DOE organizations — the Office of Science and the National Nuclear Security Administration — that brings together multiple national laboratories to develop a productive exascale capability in the U.S. by 2021. Led by Paul Messina, Argonne Distinguished Fellow and former ALCF Director of Science, the ECP's mission is to build an ecosystem that encompasses applications, system software, hardware technologies, architectures, and workforce development to pave the way for the nation's first exascale systems.

ALCF experts and computing resources will play significant roles in helping the ECP achieve its goals. Several ALCF researchers are already engaged in ECP-funded projects in application development, software development, and hardware technology. The program will also support the operation of two additional Theta racks, allowing ECP researchers to use the ALCF's leading-edge system to pursue development work at a large scale.

EXASCALE COMPUTING PROJECT

ACCELERATING EXASCALE



In the workforce development space, the ECP now funds the annual Argonne Training Program on Extreme-Scale Computing (ATPESC), which is organized and managed by ALCF staff. ATPESC is an intensive, two-week program that introduces attendees to the key skills and tools needed to carry out computational science and engineering research on leading-edge supercomputers and the extreme-scale systems of the future.

Ultimately, the ALCF and other DOE computing facilities will handle the procurement of future exascale-class supercomputers. Part of the ECP's role is to bridge and align the resources of DOE laboratories, allowing them to work more effectively with industry. This includes integration with technology and system vendors and software and application developers that goes beyond the specific needs and charters of any one laboratory. Prior to the procurement phase, the ECP will leverage its research and development work to establish the design, performance, and implementation requirements that will help shape the laboratories' exascale Request for Proposal documents.

SHAPING THE FUTURE

EVALUATING FUTURE COMPUTING TECHNOLOGIES

Argonne's Joint Laboratory for System Evaluation (JLSE) is designed to help researchers assess and improve future extreme-scale computing technologies and systems of interest to the DOE.

Established by the ALCF and Argonne's Mathematics and Computer Science Division, the JLSE was created to centralize Argonne's research activities aimed at evaluating future extreme-scale computing systems and technologies.

JLSE users from both divisions leverage existing infrastructure and next-generation hardware and software to explore low-level experimental computer and computational science, including operating systems, messaging, compilers, benchmarking, power measurements, I/O, and new file systems.

By providing access to leading-edge computing resources and fostering collaborative research, the JLSE is allowing researchers to address Argonne and DOE needs in a variety of areas, including:

- Improving science productivity on future hardware and software platforms
- Providing an avenue for Argonne researchers to work collaboratively with HPC vendors on prototype technologies for petascale and beyond
- Investigating alternative approaches to current and future system deployments
- Maintaining a range of hardware and software environments for testing research ideas
- Helping to drive standards on benchmarks, programming models, programming languages, memory technologies, etc.

For the ALCF, JLSE resources are enabling staff members to better prepare for the architecture of future systems. For example, ALCF researchers are using JLSE computing systems to analyze important application benchmarks and mini-apps to shed light on the performance and characteristics of next-generation platforms.

By considering architectural characteristics, such as instruction issue rates, memory and cache hierarchy, and vector instruction operations, the researchers are working to identify the capabilities and limitations of future architectures, best practices for improving the performance of applications, and, ultimately, a roadmap for users to effectively adapt and tune their codes for new leadership-class systems.

JLSE PROJECTS

In 2016, the JLSE supported more than 75 Argonne users participating in over 30 projects. The following summaries represent a selection of current JLSE projects.

ALCF Data Science Program

Venkatram Vishwanath

Research teams from the ALCF Data Science Program are using JLSE resources to explore and improve data science techniques, such as data mining, graph analytics, machine learning, and complex and interactive workflows.

Evaluation of Neuromorphic Computing Hardware

Hal Finkel, Fangfang Xia

In collaboration with IBM, researchers are testing various use cases for neuromorphic hardware to develop an understanding of how to best train and make use of these artificial neural networks in hardware.

Exascale Deep Learning-Enabled Precision Medicine for Cancer

Rick Stevens

Using the NVIDIA DGX-1 system and other JLSE computing resources, researchers are developing the CANcer Distributed Learning Environment (CANDLE), a computational framework designed to facilitate breakthroughs in the fight against cancer.

Integration and Validation of Argo's Components

Swann Perarnau

Argo is an exascale operating system and runtime stack being developed to support extreme-scale scientific computation.

Petrel Data Service Testbed

Ian Foster, Michael E. Papka

Petrel is a pilot service for data management that allows researchers to store large-scale datasets and easily share that data with collaborators.

RAN – RAM Area Network

William E. Allcock

Researchers are working with Kove, a high-performance storage vendor, to develop a network that treats RAM as a schedulable resource. This involves moving a portion of the RAM into a pool, so that it can be scheduled and better utilized.

Testing Globus with Spectra Logic BlackPearl

Ian Foster

The project team is working with Spectra Logic to provide a turn-key research data storage solution by developing and testing a Globus interface for the vendor's BlackPearl object storage manager.

Theta Early Science Program

Tim Williams

Theta Early Science Program teams used the Intel® Xeon Phi™ Knights Landing cluster and other JLSE resources to prepare and optimize applications for Theta in advance of the system being available.

JLSE TESTBEDS

JLSE users' research and development work is enabled by the joint lab's diverse testbeds, which include:

- Intel® Xeon Phi™ Knights Landing Cluster
- Cray Urika-GX Analytics Platform
- BM Power System S822LC
- AppliedMicro X-C1 Server Development Kit Plus
- NVIDIA DGX-1
- IBM Elastic Storage Server GL6

SHAPING THE FUTURE

ALCF'S NEW DATA SCIENCE PROGRAM TARGETS BIG DATA

With its pioneering Data Science Program, the ALCF is growing a community of users that can leverage leadership computing resources to advance data-driven discoveries.

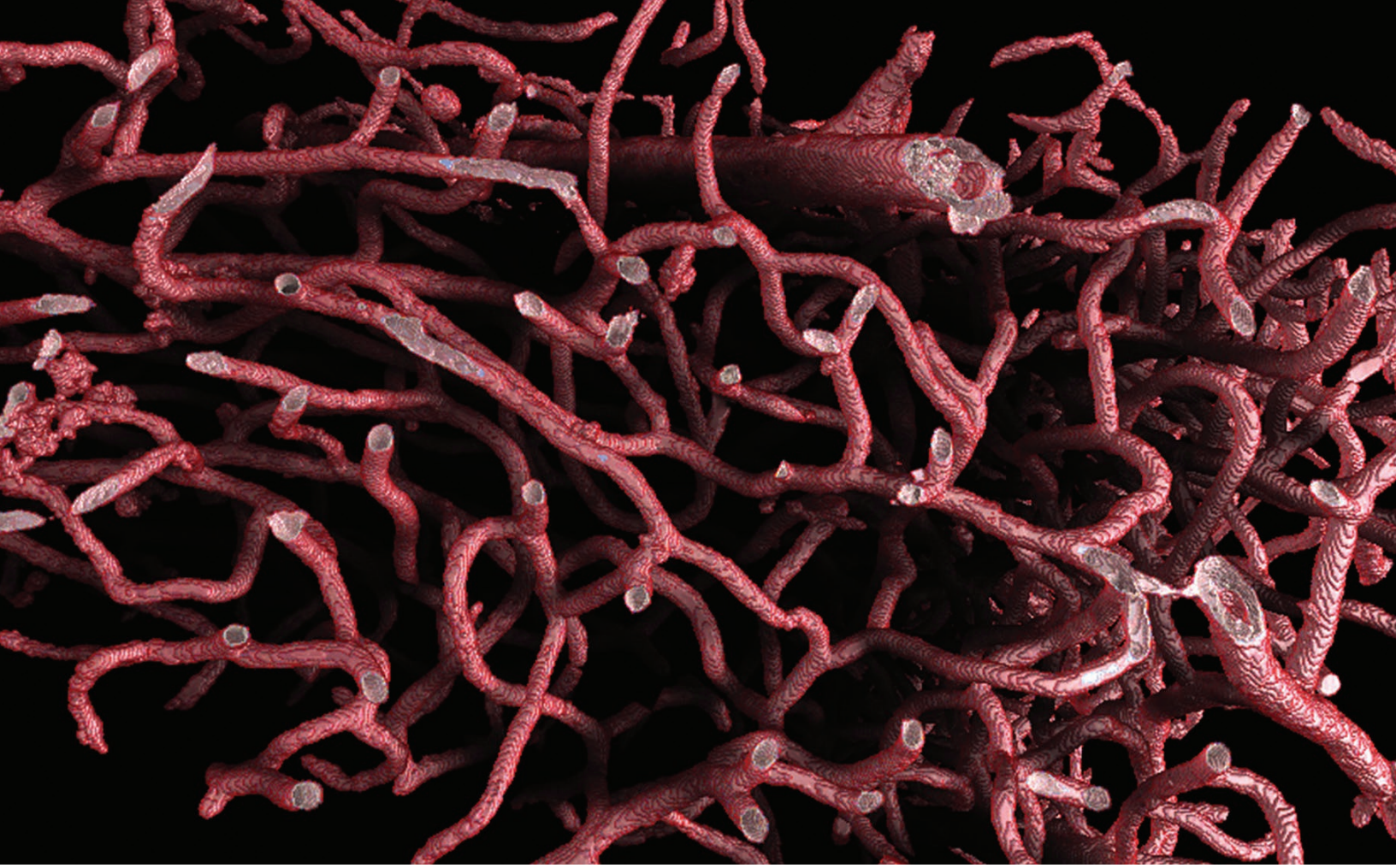
Large-scale experiments, metagenomics, urban planning, and many other data-centric application domains are generating increasingly larger amounts of data that contain scientifically significant discoveries. Leadership computing resources are massively powerful platforms that can be used to parse and analyze this data — provided the right tools and techniques can be developed, proved, and improved.

Launched in 2016, the ALCF Data Science Program (ADSP) was created to grow a community of users that are capable of using leadership-class supercomputers to advance data science across all scientific disciplines. The pioneering initiative is targeted at "big data" science problems that require the scale and performance of ALCF computing resources.

The program is allowing researchers to explore and improve a variety of computational methods and novel usage modalities that will help enable new data-driven discoveries. By developing and demonstrating rapid analysis techniques, such as data mining, graph analytics, and machine learning, together with workflows that will facilitate productive usage on extreme-scale computing systems, ADSP will help pave the way for more researchers to use supercomputers for their big data challenges in the future.

For the program's first year, the ALCF selected four projects that span experimental and computational sciences and range from physics to neuroscience. The projects, which have access to ALCF computing resources and staff, are split into two tiers, with the tier 1 projects receiving additional support from postdoctoral researchers.

ADSP teams will be among the first to access Theta, the ALCF's new Intel-Cray system. Additional computing resources for this work include Mira, Cooley, and Sage, a Cray Urika-GX analytics platform housed in Argonne's Joint Laboratory for System Evaluation.



Visualization of vessels in a mouse brain, segmented from x-ray images collected at Argonne's Advanced Photon Source.
Image credit: Joseph A. Insley and Bobby Kasthuri, Argonne National Laboratory

Advancing the Scalability of LHC Workflows to Enable Discoveries at the Energy Frontier

Taylor Childers, Argonne National Laboratory

This project will develop an end-to-end workflow managing the data motion and payload execution of the ATLAS detector simulations on ADSP resources. This would increase the analysis reach of LHC scientists, enabling new discoveries in particle physics.

Data-Driven Molecular Engineering of Solar-Powered Windows

Jacqueline Cole, University of Cambridge

This project aims to develop a new material-by-design methodology by using machine learning and data mining in conjunction with large-scale simulations and experiments. This synergistic computational and experimental science approach will enable the discovery of new light-absorbing dye molecules, which are needed for the development of solar-powered windows that have the potential to power buildings in an entirely energy-sustainable fashion.

Large-Scale Computing and Visualization on the Connectomes of the Brain

Doga Gursoy, Argonne National Laboratory

This project's objective is to enable extreme-scale, data-centric pipelines for brain science. The scalable workflows, focused on analysis and visualization of experimental data, will help researchers gain invaluable knowledge about disease models, such as Alzheimer's, autism spectrum disorder, and many others. Additionally, the insights gleaned will enable transformative advances in neuromorphic computing.

Leveraging Non-Volatile Memory, Big Data, and Distributed Workflow Technology to Leap Forward Brain Modeling

Fabien Delalondre, Blue Brain Project, EPFL

The goal of this project is to facilitate and support complex computational neuroscience workflows through the integration of new data storage paradigms, run times, and big data technology. This will enable the simulation and analysis of brain tissue models at unprecedented scales, paving the way for future brain research and neuroscience breakthroughs.

SHAPING THE FUTURE

DRIVING INNOVATION AND COMPETITIVENESS FOR U.S. INDUSTRY

Industry partnerships with the ALCF help to strengthen the nation's innovation infrastructure and expand the use of supercomputing resources for national competitiveness.

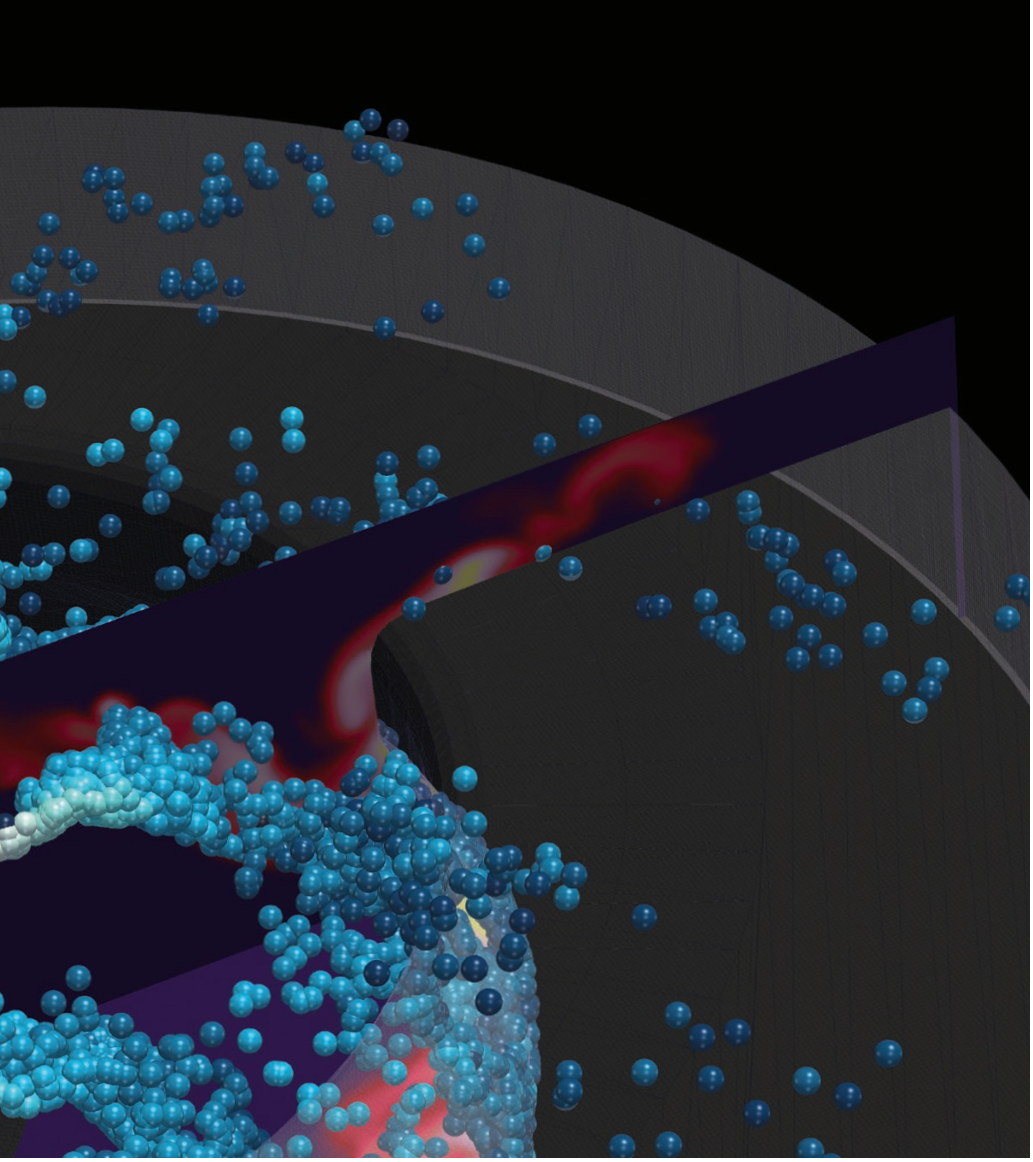
The ALCF's industrial outreach efforts aim to grow the facility's base of industry users by identifying prospective companies of all sizes, from start-ups to Fortune 500 corporations, that could benefit from leadership computing resources and collaborative opportunities with the ALCF and across Argonne.

Supercomputers like Mira enable U.S. companies to tackle computational problems that are impossible to address on most internal computing systems. Access to ALCF computing systems gives them the ability to perform more complex simulations, achieve more accurate predictions, and create higher fidelity models of everything from battery materials to combustion.

The results allow companies to accelerate critical breakthroughs, verify uncertainties, and drastically reduce or eliminate the need to build multiple prototypes. Ultimately, industry partnerships with the ALCF help to strengthen the nation's innovation infrastructure and expand the use of HPC resources for national competitiveness.

In addition to gaining access to some of the world's most powerful supercomputers, industry users also benefit from the ALCF's expertise in novel computational methods and algorithms, application porting, performance tuning and scaling, and data analysis and visualization.

The ALCF has recently enhanced its industry outreach program by partnering with other Argonne user facilities and divisions, including the Technology Development and Commercialization Division. This collaborative approach allows the ALCF to present a more complete picture of the laboratory's resources and encourages additional collaborations. These efforts have resulted in broader engagements across the laboratory with a number of companies.



High-fidelity 3D simulations provide unique insights into the development of next-generation engines. This simulation captures fuel distribution inside the combustion chamber of a GM 1.9 L diesel engine being operated in a novel low-temperature combustion mode developed at Argonne.

Image credit: Joseph A. Insley, Janardhan Kodavasal, and Sibendu Som, Argonne National Laboratory

Brewer Science Seeks to Develop New Materials for Semiconductor Industry

Brewer Science brings innovative material technologies, process solutions, manufacturing, and metrology capabilities to advance various industries such as semiconductor, electronics packaging, and printed electronics. The company formed a multifaceted partnership with the ALCF and other Argonne divisions to advance their work with new material platforms, enabling multilayer lithography patterning and directed self-assembly applications. Brewer Science's ultimate goal is to use supercomputers to better understand the codependence of structure-property relationships of new polymer-based compositions, providing insights to guide the development of materials that will benefit the semiconductor industry.

Convergent Science Uses Supercomputers to Improve Virtual Engine Design

Researchers from Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI) are working with ALCF staff and Convergent Science Inc. to optimize the CONVERGE code, a commercial computational fluid dynamics (CFD) software tool, for Mira. This ongoing collaboration aims to develop HPC engine modeling and simulation capabilities, providing U.S. automotive manufacturers with a cost-effective tool to accelerate the development of more energy-efficient engines. Such tools have the potential to improve the fuel economy of vehicles, thereby reducing U.S. dependence on foreign oil and reducing carbon emissions.

GE Performs Simulations to Guide the Design of Better Aircraft Engines

The aviation industry demands each generation of engines powering modern aircraft improve fuel efficiency while meeting environmental regulations. Pursuing insights toward better designs, GE researchers, in partnership with Cascade Technologies, are using ALCF supercomputers to study the complex physics of an engine's combustor liner flows. Findings from this project will provide high-fidelity datasets to guide the low-fidelity models currently available to engine designers. Ultimately, the results will help engineers design and optimize competitive aircraft engines that deliver better fuel efficiency, lower emissions, and improved performance.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COMMUNITY & OUTREACH

As a leader in the HPC community, the ALCF is actively involved in efforts to broaden the impact of supercomputers and grow the community of researchers who can use them for computational science and engineering research.

ALCF staff members Jini Ramprakash and Beth Cerny (right) give students a tour of the facility's machine room as part of Argonne's annual Science Careers in Search of Women conference.

Argonne Associate Laboratory Director Rick Stevens addresses researchers at the 2016 Intel® Xeon Phi™ User's Group (IXPUG) annual meeting.

PROPELLING THE HPC COMMUNITY

ALCF researchers are engaged in many forward-looking activities aimed at advancing the use of supercomputers for discovery and innovation.

Accelerating the Search for New Physics

Physicists from across the country visited Argonne National Laboratory in April for a two-day workshop designed to generate new ideas and projects that will advance breakthroughs in physics. Sponsored by the ALCF and Lawrence Livermore National Laboratory, the Lattice for Beyond the Standard Model Physics 2016 workshop brought together the computational, phenomenological, and experimental communities to present recent findings and explore opportunities for collaboration. The focus of this year's workshop was on the role that lattice numerical simulations can play in the search for physics beyond the Standard Model.

Advancing the QMC Method

The quantum Monte Carlo (QMC) method is one of the most accurate electronic structure methods, providing an important computational tool for performing many-body calculations for a broad range of electronic systems. In 2016, the ALCF was named an Intel Parallel Computing Center for QMCPACK, a high-performance, open-source QMC code. Bringing together researchers from ALCF, Sandia National Laboratories, and Intel, the center is focused on optimizing QMCPACK for the next-generation Intel® Xeon Phi™ computing architectures that will be going online at several DOE supercomputing centers in the coming years. In a separate effort to advance QMC research, ALCF staff and computing resources supported the 2016 QMC Workshop, a weeklong, hands-on training event at the University of Illinois at Urbana-Champaign that introduced attendees to the fundamentals of QMC theory, and recent developments in methods and applications in physics, chemistry, and materials sciences.

ALCF Deputy Director of Science Tim Williams (center) participates in a panel discussion on earlyexperiences with the Intel® Xeon Phi™ processor at the 2016 IXPUG annual meeting.

Identifying DOE Requirements for Exascale

For the past two years, the ALCF has collaborated with its fellow DOE ASCR facilities to conduct a series of Exascale Requirements Reviews to determine the mission-critical computational science objectives for each of the six DOE Office of Science program offices through 2025. These workshops brought together key domain scientists and computational science experts to identify the requirements for developing an exascale ecosystem that includes computation, data analysis, software, workflows, HPC services, and other features. ALCF staff members, in collaboration with Argonne's Communications, Education, and Public Affairs Division, were also responsible for managing and producing the final reports from each of the six reviews, as well as developing and maintaining the Exascale Requirements Reviews website (exascale.org).

Illuminating the Intel Xeon Phi Processor

In September, Argonne National Laboratory hosted the Intel® Xeon Phi™ User's Group's (IXPUG) 2016 annual meeting, which welcomed more than 130 researchers from around the world for four days of tutorials, workshops, and talks on the Intel® Xeon Phi™ processor. The ALCF's next-generation supercomputers, Aurora and Theta, are based on successive generations of the Intel processor. As one of the founding members of IXPUG, the ALCF has been active in the group's mission to provide a forum for exchanging information to enhance the usability and efficiency of scientific and technical applications running on large-scale HPC systems that use the new processor.

Showcasing HPC Capabilities for Engine R&D

As a partner in Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI), the ALCF played a key role in VERIFI's 2016 workshop on the role of simulations and high-performance computing in engines and fuels co-optimization. Held at the laboratory in June, the two-day workshop welcomed several representatives from the automotive industry for guidance on how VERIFI and the ALCF can help accelerate R&D efforts related to next-generation engines and fuels. In addition to showcasing current methodologies and capabilities, ALCF staff facilitated a hands-on session with Mira to demonstrate how supercomputers can be used to quickly run a series of practical engine simulations.

The ALCF is committed to providing training and outreach opportunities that prepare researchers to efficiently use its leadership computing systems, while also cultivating a diverse and skilled HPC workforce for the future.

ENGAGING CURRENT AND FUTURE USERS

The 2016 Argonne Training Program on Extreme-Scale Computing brought together 65 participants for two weeks of instruction on the tools and approaches needed to use the world's most powerful supercomputers for science and engineering research.

INSPIRING STUDENTS

Computational Science Coursework

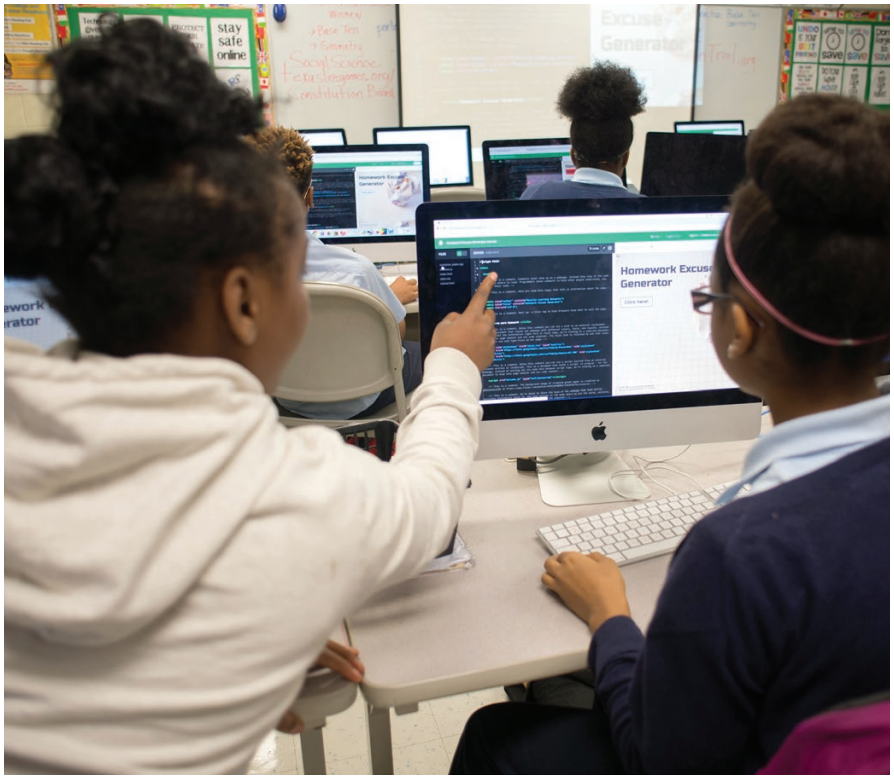
ALCF staff played a large role in organizing and executing the Harvard University graduate course Extreme Computing: Project-Based High Performance Distributed and Parallel Systems. This applied computation course, part of a category of courses developed by Harvard's Institute of Applied Computational Science, highlighted the use of supercomputers to solve scientific problems and provided hands-on lessons, which included running jobs on Mira.

Hour of Code

As part of Code.org's annual Hour of Code event in December, several ALCF staff members visited Chicago-area schools to spark interest in computer science and coding. Working with classrooms ranging from kindergarten to high school, the ALCF volunteers led a variety of activities designed to demystify code and show that anybody can learn the basics. The global outreach campaign aims to expand participation and increase diversity in computer science.

Promoting STEM Careers to Young Women

Through participation in Argonne events like Introduce a Girl to Engineering Day and the Science Careers in Search of Women conference, ALCF staff members have the opportunity to connect with young women and introduce them to potential career paths in science, technology, engineering, and mathematics (STEM). The ALCF also promotes STEM careers to women through contributions to Argonne's Women in Science and Technology group, the Anita Borg Institute, the Grace Hopper Celebration of Women in Computing, and the Rocky Mountain Celebration of Women in Computing.



Several ALCF staff members volunteered to lead Hour of Code activities in K-12 classrooms as part of Computer Science Education Week in December.

Summer Coding Camp

For the past two years, ALCF staff members have teamed with Argonne's education office to host an intensive coding camp for Chicago-area high school students. The weeklong course, developed and delivered by ALCF computer scientists, emphasized problem-solving skills and hands-on activities, including coding in Python and using a Raspberry Pi to program a robot.

Summer Student Program

In 2016, 22 students from universities around the country spent their summer at the ALCF, tackling a wide variety of projects that covered everything from HPC system administration and data analytics to computational science and performance engineering. Every year, the facility solicits student project proposals from staff members who are interested in mentoring summer students. Through programs like DOE's Science Undergraduate Laboratory Internship program and Argonne's Research Aide Appointments, college students, ranging from freshmen to PhD candidates, are brought in to work alongside ALCF mentors on real-world research projects. The program culminates with a special symposium in which the students present their project results.

The ALCF's annual hands-on workshop provides an opportunity for users to work directly with ALCF staff to test, debug, and improve their codes.

TRAINING USERS

Annual Hands-On Workshop

In May, the ALCF's annual hands-on workshop, Scaling Your Science on Mira, welcomed both prospective and current users to work directly with ALCF computational scientists and industry experts on testing, debugging, and improving their codes on the facility's IBM Blue Gene/Q supercomputer. One of the workshop's goals is to help researchers demonstrate code scalability for a future allocation award at the ALCF. The two primary allocation programs for DOE leadership computing resources — INCITE and ALCC — require project proposals to convey both scientific merit and computational readiness. The ALCF's hands-on workshop is a key resource for many teams seeking to fulfill the latter requirement. Current ALCF users also attend the annual workshop to learn tips and techniques for maximizing their time on the facility's systems. In addition to hands-on sessions, the event featured talks on the IBM Blue Gene/Q architecture, parallel I/O, data analysis, and various HPC tools.

ATPESC

Now in its fourth year, the Argonne Training Program on Extreme-Scale Computing (ATPESC) is designed to teach participants the key skills and tools needed to efficiently use leading-edge supercomputers. Developed and managed by ALCF staff, the rigorous training program brought 65 graduates, postdocs, and researchers together at the Pheasant Run Resort in St. Charles, Illinois, in August, for two weeks of instruction on HPC codes, software, and architecture. As with previous years, all of the 2016 ATPESC presentations were recorded and posted to YouTube to extend the reach of the program. ATPESC is now funded by the Exascale Computing Project, a collaborative effort of the DOE Office of Science and the National Nuclear Security Administration.

Best Practices for HPC Software Developers

In 2016, the ALCF, the Oak Ridge Leadership Computing Facility, the National Energy Research Scientific Computing Center, and the Interoperable Design of Extreme-Scale Application Software (IDEAS) project launched a series of webinars — Best Practices for HPC Software Developers — to help users of HPC systems carry out their software development more productively.

Cray Urika-GX Training

With the launch of a Cray Urika-GX system this fall, Argonne National Laboratory became the first research center to deploy the new computing platform for big data analytics. In December, a group of 38 researchers gathered at the laboratory to learn how the system, named Sage, can help advance their data-intensive science problems. Hosted by the ALCF, the two-day workshop, led by experts from Cray, provided an overview of the new system's features and capabilities, and an opportunity for collaborative, hands-on training sessions. Sage, which is housed in Argonne's Joint Laboratory for System Evaluation, is one of the computing resources available to researchers participating in the ALCF Data Science Program.

In December, the ALCF hosted a two-day workshop to introduce a group of researchers to Sage, Argonne's new Cray Urika-GX platform.

From introducing students to exciting career possibilities in HPC to working with users to inform them of new approaches for leadership-class systems, education is a critical part of the ALCF's mission.

Theta ESP Workshop

In August, the ALCF hosted researchers from its Theta Early Science Program (ESP) for a hands-on workshop to help them port, benchmark, and optimize their applications on the facility's next-generation Intel-Cray system. The four-day workshop included instruction from ALCF, Intel, and Cray staff on various tools and tips for running on Theta, and collaborative sessions aimed at getting the research teams' codes running on the actual machine.

The ALCF's hands-on workshop is a key resource for researchers seeking to demonstrate code scalability for project proposals.

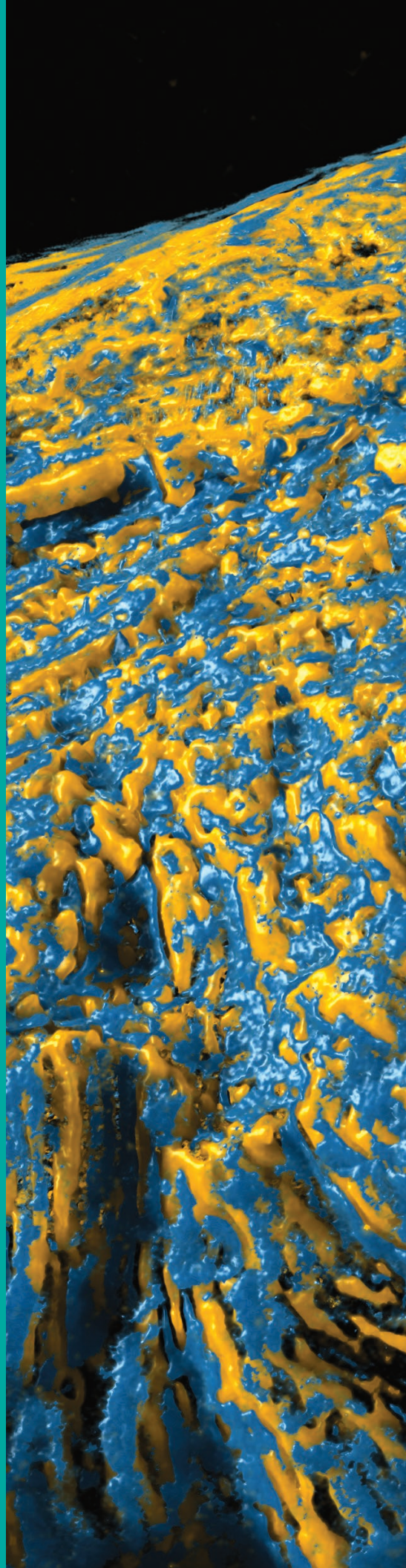
Virtual Training

Employing an interactive videoconference format, the ALCF is able to connect with users from around the globe to provide virtual training on ALCF services and resources. Offered several times a year, the Getting Started on ALCF Resources videoconference is targeted at new users and those in need of a refresher. The highly interactive sessions cover the basics that researchers need to get their projects up and running, and give users an opportunity to receive guided assistance in building their codes and submitting jobs on Mira.

The ALCF also uses the virtual format for its Ensemble Jobs for Better Throughput videoconference. This specialized training session provides hands-on experience setting up an ensemble job script and helps users identify which job submission type is best for their projects.

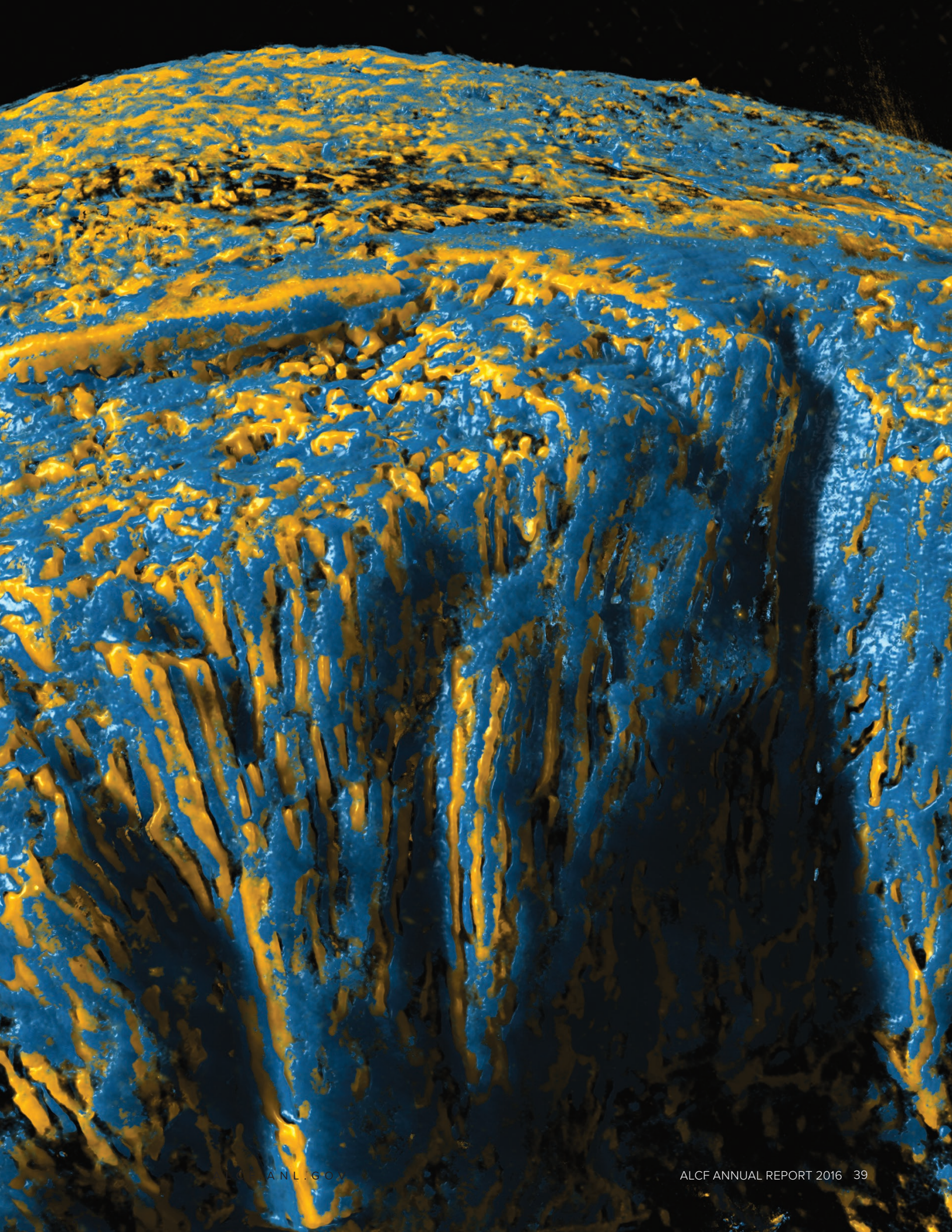
SCIENCE

The ALCF is accelerating scientific discoveries in many disciplines, ranging from chemistry and engineering to physics and materials science.



A research team from Argonne National Laboratory and the University of Chicago is using nanometer-scale imagery of the enamel of a primate tooth to study its internal structure and test hypotheses related to mechanical characteristics. The data was imaged using high-resolution x-ray tomography at Argonne's Advanced Photon Source. To analyze the inherent structures of these large-scale experimental datasets, the team worked with ALCF researchers to visualize the data using the vl3 parallel volume rendering framework.

Image credit: James Grudzinski, Carmen Soriano Hoyuelos, Joseph A. Insley, and Silvio Rizzi, Argonne National Laboratory; Callum Ross, The University of Chicago

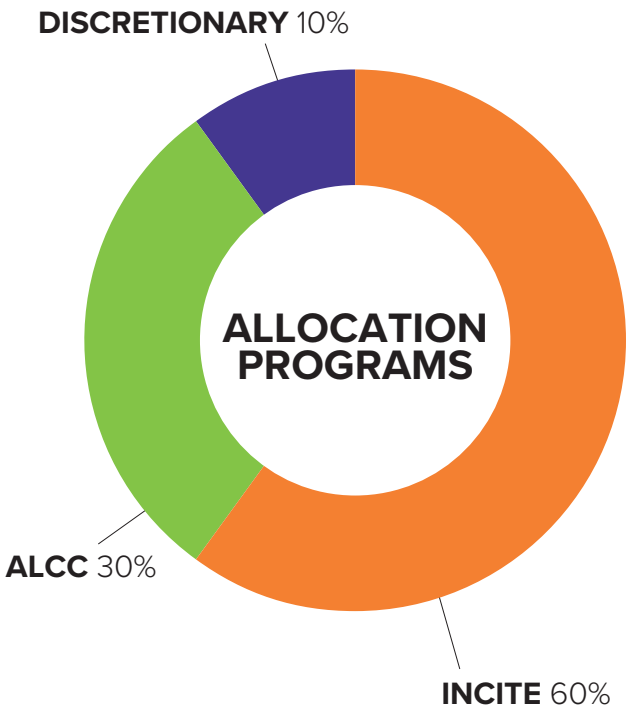


ACCESSING ALCF RESOURCES

As a national user facility dedicated to open science, any researcher in the world with a large-scale computing problem can apply for time on ALCF computing resources.

Researchers gain access to ALCF systems for computational science and engineering projects, typically with awards of millions of core-hours, through competitive, peer-reviewed allocations programs supported by the DOE and Argonne.

The ALCF also hosts competitive, peer-reviewed application programs designed to prepare key scientific applications and innovative computational methods for the architecture and scale of ALCF supercomputers.



A breakdown of how computing time on Mira is allotted among the three allocation programs.

APPLICATION PROGRAMS

Early Science Program (ESP)

As part of the process of bringing a new supercomputer into production, the ALCF hosts the ESP to ensure its next-generation systems are ready for science on day one.

ALCF Data Science Program (ADSP)

Targeted at big data science problems, ADSP aims to explore and improve a variety of computational methods that will help enable data-driven discoveries across all scientific disciplines.

ALLOCATION PROGRAMS

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

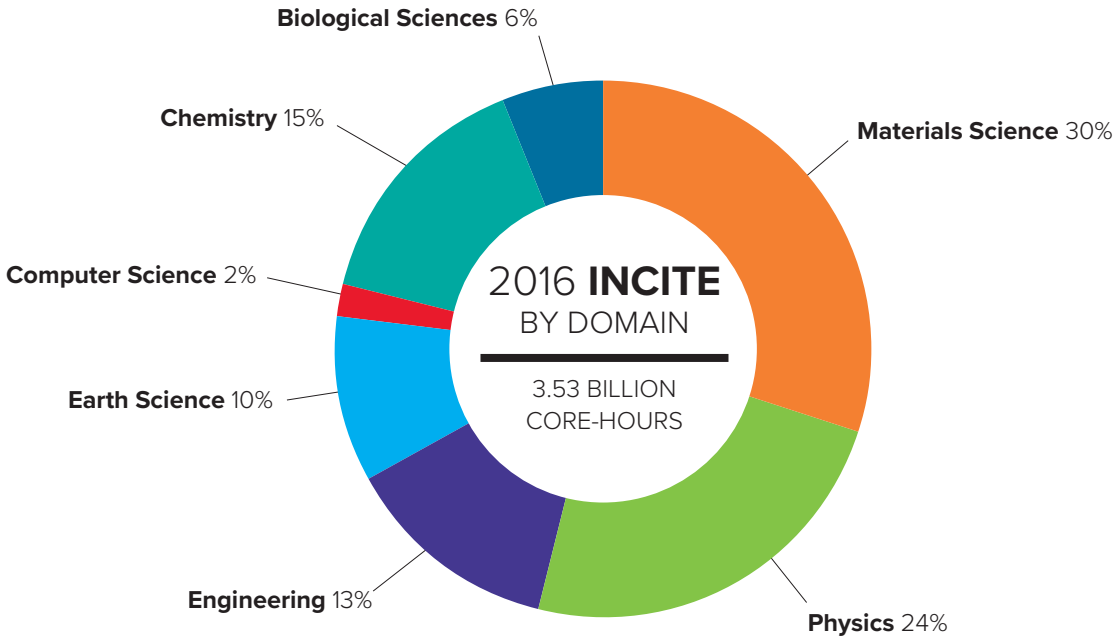
The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering.

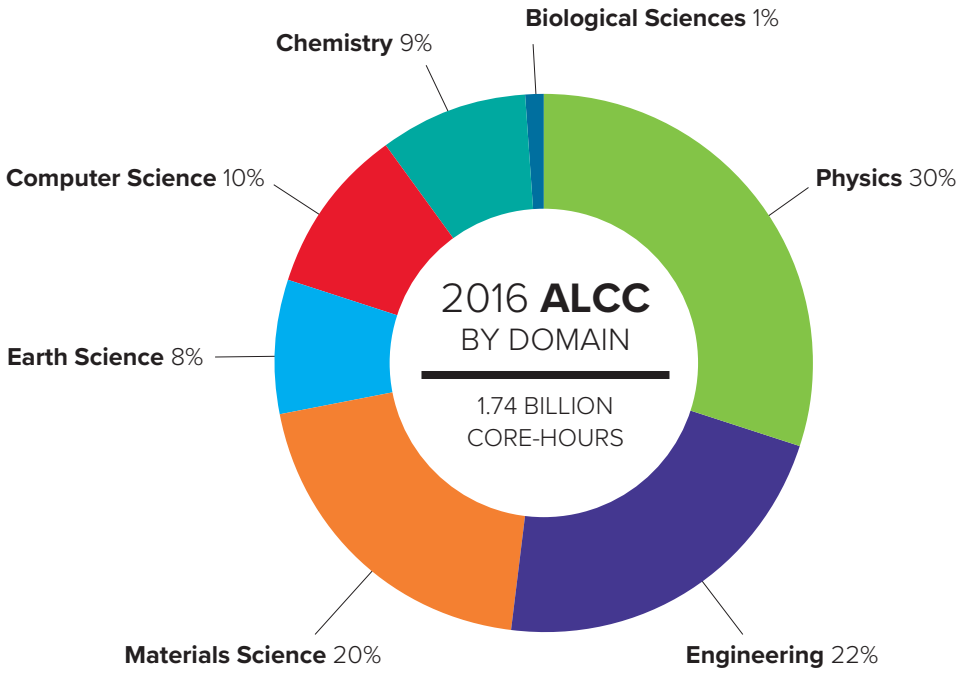
ASCR Leadership Computing Challenge (ALCC)

The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, as well as national emergencies, and for broadening the community of researchers capable of using leadership computing resources.

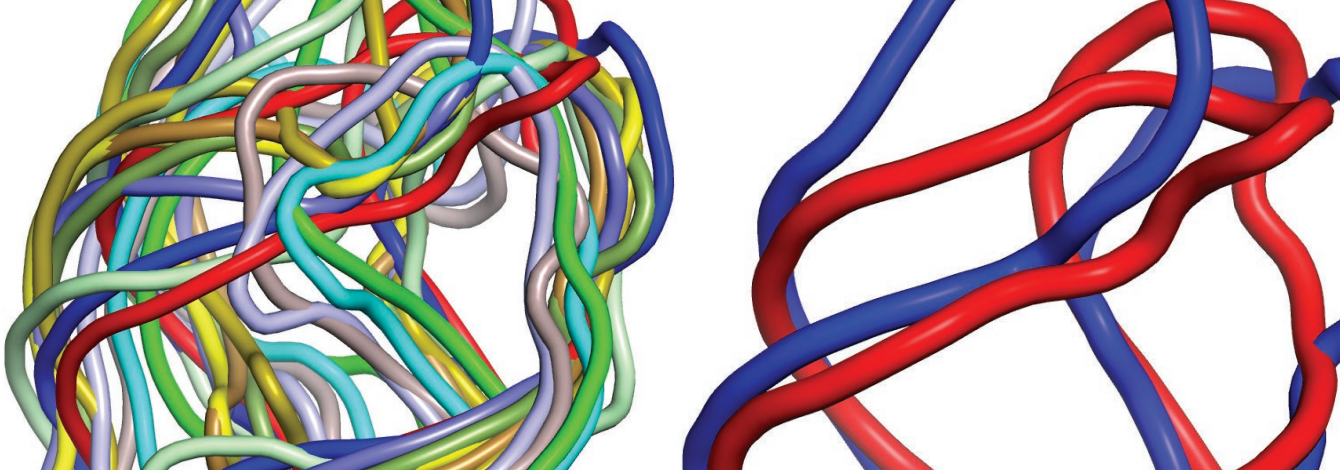
Director's Discretionary

The ALCF's Director's Discretionary program provides "start-up" awards to researchers working toward an INCITE or ALCC allocation to help them achieve computational readiness.





Note: ALCC data is from calendar year 2016.



COMPUTING 3D STRUCTURES OF RNA FROM SMALL-ANGLE X-RAY SCATTERING DATA AND SECONDARY STRUCTURES

YUBA BHANDARI
bhandariyr@mail.nih.gov

YUN-XING WANG
wangyunx@mail.nih.gov
National Cancer Institute

Director's Discretionary

15 Million Core-Hours
Biological Sciences

Ribonucleic acid (RNA) plays a critical role in regulating cellular processes, making it an important area of research for cancer studies. Gaining a better understanding of RNA depends on knowledge of its 3D structures, but such structures are difficult to ascertain with conventional methods. Researchers from the National Cancer Institute are using ALCF computing resources to develop a novel approach for calculating RNA structures that would greatly improve our understanding of RNA biology.

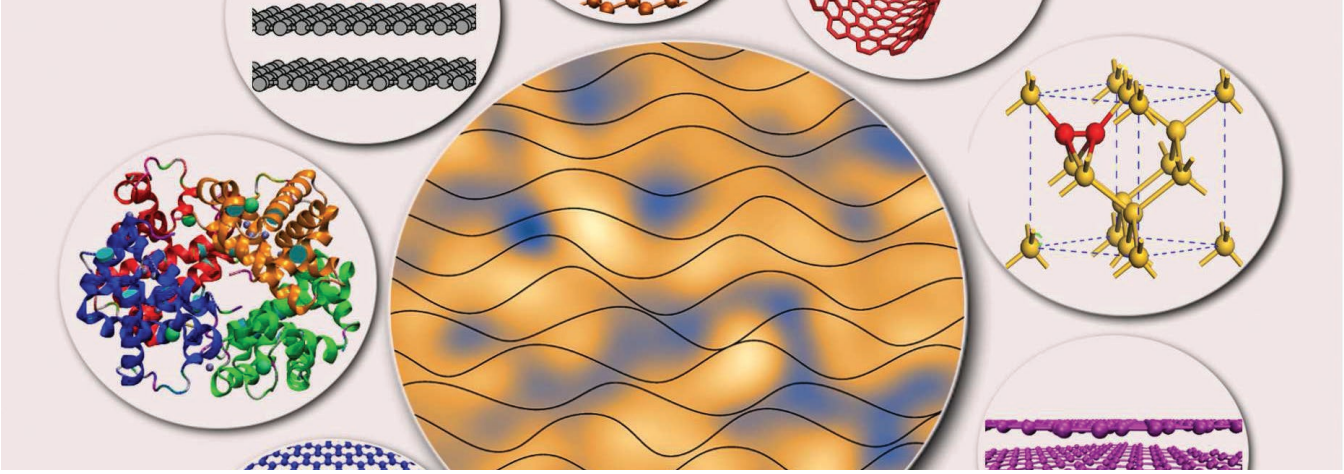
APPROACH The research team developed a robust algorithm and computational program called RS3D to calculate 3D structures of RNA using small-angle x-ray scattering (SAXS) data and known secondary structures as input. Starting from a glob model at nucleotide level of resolution, the algorithm carries out natural hierarchical moves based on the structural composition of RNA. Each move is guided toward improving the SAXS data fit and long-range interactions, if available. To conduct these types of calculations, the researchers must generate tens of thousands of structures for each type of RNA. Computing the RNA structures with various folds and complexities necessitates the use of a petascale supercomputer like Mira. In collaboration with ALCF researchers, the team has scaled and optimized RS3D to improve its performance on Mira.

RESULTS The team published a paper in the journal *Methods* detailing their computational approach to model RNA structures using SAXS data. They also validated the RS3D method extensively, using more than 15 different RNA structures that represent a wide variety of folding architectures available in the current structural database. By computing 3D topological RNA structures with diverse junction types and structural complexities, the team demonstrated the utility and robustness of RS3D, using simulated as well as experimental SAXS data. The method's novel features include conceptual simplicity that incorporates secondary structure motifs and the flexibility to integrate a variety of tertiary interactions that users can obtain from biochemical and biophysical data.

IMPACT This project is developing a high-throughput method that can determine the structure of RNA in a diverse folding landscape to fill in the gap between known RNA sequences and their explicit 3D structures. This work has significant implications in understanding the structural basis of RNA biology, and thus in the advancement of RNA therapeutics.

Image: Explicit 3D structures of adenine riboswitch RNA (PDB ID 1Y26) calculated using the RS3D program.

Image credit: Wei Jiang, Argonne National Laboratory; Yuba Bhandari and Yun-Xing Wang, National Cancer Institute



ANOMALOUS DENSITY PROPERTIES AND ION SOLVATION IN LIQUID WATER: A PATH-INTEGRAL AB INITIO STUDY

ROBERT A. DISTASIO

distasio@cornell.edu
Cornell University

ALCC

175 Million Core-Hours
Chemistry

Image: Researchers used Mira to validate a new many-body "wave-like" theoretical model to accurately solve for the van der Waals forces, demonstrating that this long-range interaction can be significantly enhanced at the nanoscale. This discovery is one component of the team's work, which involves carrying out large-scale simulations of liquid.

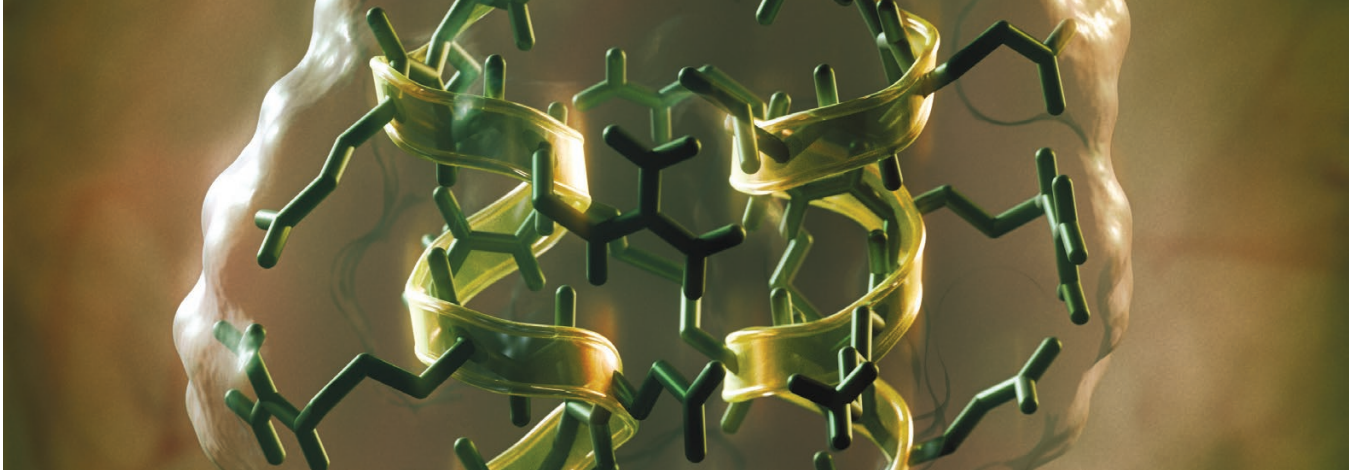
Image credit: Robert A. DiStasio, Cornell University; Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society and University of Luxembourg

Water is essential to life and critical to research fields addressing some of today's biggest energy challenges. Although the structure of a single water molecule is known, liquid water has a complex, disordered microscopic structure that is difficult to observe. At present, there is no experimental method that can probe the microscopic structure of liquid water, and many computer-based simulations, though useful for other types of microscopic molecular modeling, cannot reproduce the structure and dynamics of water and aqueous solutions important to applications, such as industrial catalysts, fuel cells, and protein stability.

APPROACH Researchers from Cornell and Princeton are performing highly accurate benchmark atomistic simulations of liquid water and aqueous ionic solutions through a combination of algorithmic advances and high-performance computing. The team has conducted large-scale simulations of liquid water, pyridine, and pyridine-like molecular crystals that are found in processes like DNA synthesis; and hydronium and hydroxide aqueous ionic solutions that provide fundamental models of acidic and basic conditions. Researchers are using the electronic structure code Quantum ESPRESSO (QE) to perform *ab initio* molecular dynamics simulations utilizing density functional theory. ALCF staff helped improve the performance of QE simulations up to 40 percent by making better use of Mira's processors and reducing interprocessor communication.

RESULTS Results include a highly accurate characterization of microscopic structures and anomalous density properties of liquid water and crystalline ice; proton transfer rates and diffusivities of aqueous hydronium and hydroxide ions; and new insights into how the long-range van der Waals interactions and nuclear quantum effects affect the structure and equilibrium densities of pyridine and pyridine-like crystals. Related to the latter finding, the team recently validated a new "wave-like" theoretical model of the van der Waals force that better predicts how it behaves at the nanoscale. The results were published in the journal *Science* in 2016.

IMPACT For this project, researchers are simulating the microscopic structure and equilibrium properties of liquid water and aqueous ionic solutions with unprecedented accuracy, addressing important areas of renewable energy research, such as the design of aqueous ion batteries and fuel cells.



TOWARDS BREAKTHROUGHS IN PROTEIN STRUCTURE CALCULATION AND DESIGN

DAVID BAKER

dabaker@u.washington.edu
University of Washington

INCITE

120 Million Core-Hours
Chemistry

Image: This man-made peptide contains both natural and mirror-image amino acid building blocks. This arrangement, which was modeled using Mira, gives rise to spirals that twist in opposite directions, a structure not seen in any natural proteins.

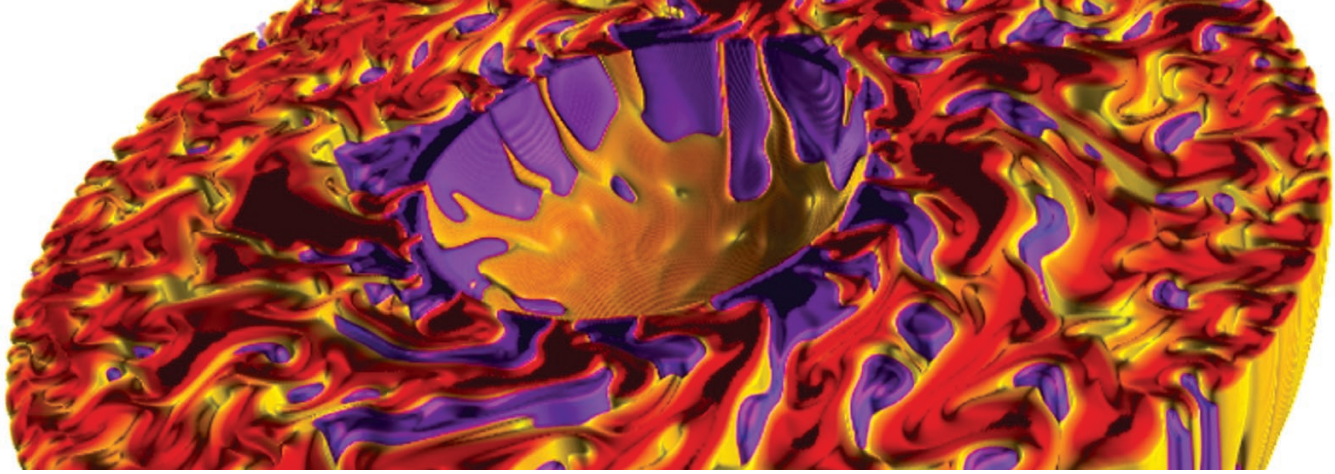
Image credit: Vikram Mulligan, University of Washington

Small-molecule drugs like aspirin use active ingredients that can cause unwanted side effects as they spread easily throughout the body. Protein drugs, designed to reduce side effects, can have the opposite problem — proteins can be too big, making it difficult to cross key membranes such as the blood-brain barrier. Researchers from the University of Washington are using Mira to develop and apply new computational methods for protein structure design, particularly that of small proteins called peptides, to further the impact of medicine.

APPROACH The Rosetta software suite, developed at the University of Washington's Baker Laboratory, is designed to tackle two difficult computational problems: the prediction of protein structure from amino acid sequences and the design of new amino acid sequences to yield a desired function. To enable the computational design work, the team developed a multistate design approach that allows them to create novel peptides with unique, rigid folds. Their method involves exhaustively enumerating the possible conformations of peptides to search for a sequence that uniquely stabilizes one desired structure and destabilizes alternative structures. The search algorithm benefits enormously from Mira's massively parallel architecture, particularly when assigning each conformational state to a separate core for simultaneous sampling.

RESULTS The team made fundamental improvements to Rosetta's high-resolution energy function, including its agreement with observational studies and ability to reproduce and discriminate amino acid sequences. Using their multistate design approach, the researchers successfully designed stable versions of synthetic peptides. They validated the computational protocol by assembling physical peptides in the laboratory, which compared remarkably well with the simulated peptides. The team detailed their results in a paper published in *Nature*.

IMPACT This project is advancing protein structure modeling capabilities to enable the design of novel proteins, including therapeutic peptides that target diseases such as Ebola, HIV, and Alzheimer's. Artificial peptides represent a new class of drugs that have potential for greater efficacy and fewer side effects. The computational tools can also be used to design peptide catalysts and enzymes for environmental, energy, and industrial applications.



FRONTIERS IN PLANETARY AND STELLAR MAGNETISM THROUGH HIGH-PERFORMANCE COMPUTING

JONATHAN AURNOU

aurnou@gmail.com
University of California, Los Angeles

INCITE

83 Million Core-Hours
Earth Science

Image: Temperature perturbations as realized in rotating, Earth-like convection at Ekman number 10-5. Warm temperature perturbations are rendered in yellow, cool in violet tones. The rendering has been cut at the equatorial plane to reveal the interior structure of convective columns that arise under such rotationally constrained conditions.

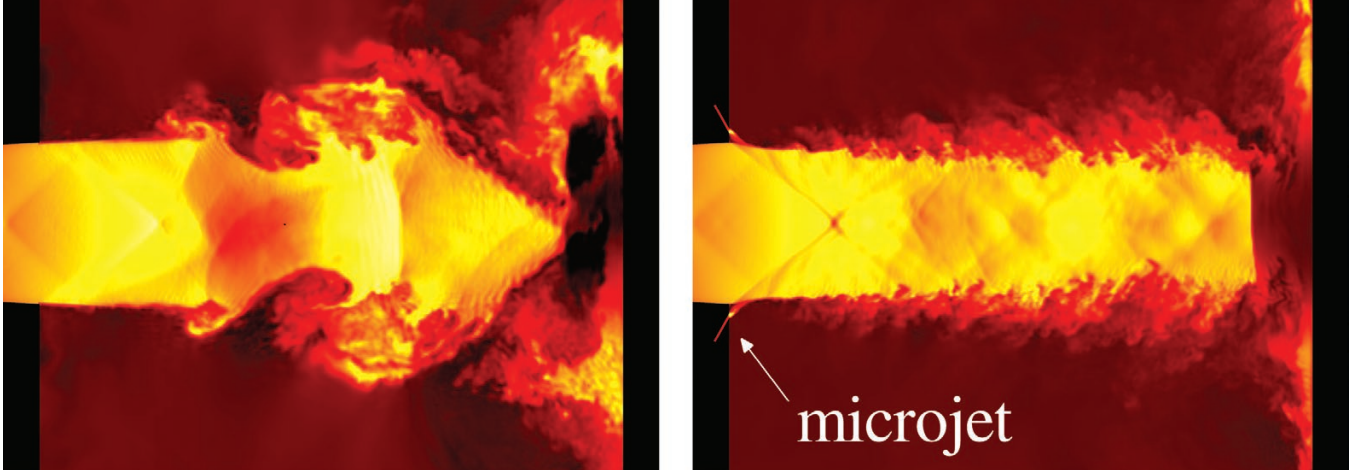
Image credit: Nicholas Featherstone, University of Colorado Boulder

Magnetic fields are generated deep within the interiors of stars and planets through dynamo action, where the motion of a conducting fluid produces an outward flux of heat. Solar and terrestrial magnetism, whether generated by iron in the Earth's core or dense plasma at the heart of the sun, plays an important role in our modern technological society, where Earth's magnetic field shields us from explosive, magnetically driven, solar phenomena. As the process of magnetic-field generation remains largely inaccessible to direct observation, researchers are leveraging ALCF computing resources to develop a new generation of models describing the dynamics at play in the Sun, Earth, and Jupiter.

APPROACH Through this ongoing investigation, a team of geo- and astrophysicists continue to develop state-of-the-art computational models to describe the interior dynamics of the Sun, Earth, and Jupiter. ALCF staff has participated in the application code development of Rayleigh, a pseudo-spectral code designed to study magnetohydrodynamic convection in spheres. Optimized to Mira, the code has allowed the team to construct high-resolution models detailing how convection transports energy generated by fusion deep within the Sun's core to the solar surface. This code and computer combination can resolve a range of spatial scales previously inaccessible to numerical simulation, ranging from the Sun's diameter to those roughly 1,000 times smaller.

RESULTS In 2016, the team added a new layer to the Rayleigh code, allowing it to solve on radially nested Chebyshev grids, which facilitates both higher accuracy and lower computational cost. While the team continues to evolve its solar simulations to include the effects of rotation on kinetic-energy scaling laws, simulations on Jovian dynamics have begun in earnest. They recently carried out the first survey to understand the appropriate internal heating functions for Jupiter simulations in preparation for primary, non-magnetic, Jupiter runs, which will constitute the highest-resolution Jupiter simulations yet.

IMPACT These models will open new windows into the understanding of the interplay of magnetism, rotation, and turbulent convection occurring within the remote interiors of geophysical and astrophysical bodies. The research will also provide the broader community access to the singular, extreme datasets generated by these massive computational efforts.



NOVEL REDUCED-ORDER MODELS OF TURBULENT JET NOISE FROM HIGH-FIDELITY SIMULATION

JOSEPH NICHOLS
jwn@umn.edu
University of Minnesota

Director's Discretionary

10 Million Core-Hours
Engineering

Image: Researchers performed high-fidelity simulations to reproduce laboratory experiments of a supersonic jet striking a flat wall (left). Analysis of reduced-order models extracted from simulations led to predictions of modified nozzle designs (right). The simulations confirmed drastically altered dynamics and low noise levels.

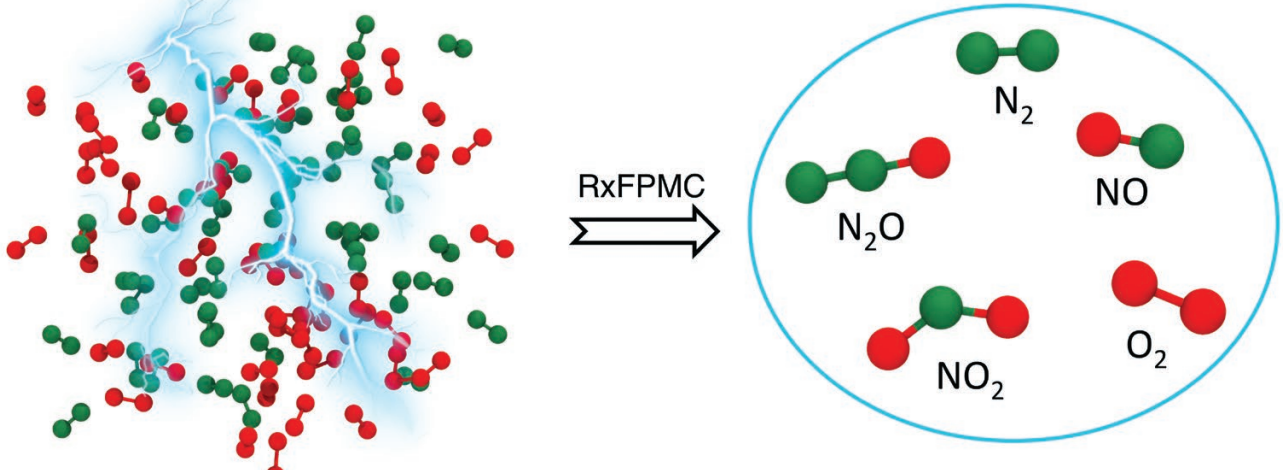
Image credit: Joseph Nichols, University of Minnesota

The reduction of noise is now an important design parameter in the research and development of jet engines. There remains, however, a lack of basic understanding of the mechanisms by which high-speed turbulent flows, like engine exhausts, generate sound. Researchers are using ALCF supercomputers to construct novel, computationally inexpensive techniques to predict and understand the aeroacoustics of high-speed jets.

APPROACH Early models of jet noise involve acoustic analogy, useful in identifying compact acoustic sources. In this framework, non-compact effects important to jet flows in and from ducts, can only be recovered by complicated two-point two-time correlations. Methods inspired by instability theory, such as the parabolized stability equations (PSE), can model non-compact acoustic sources, but do not yet fully recover the far-field acoustics of high-speed jets, especially in the sideline direction, perpendicular to the flow. Researchers applied input-output (I/O) analysis to understand the shortcomings of the PSE and to predict sound in this important direction. Taking another step, the team constructed a model of a supersonic jet that strikes a flat surface, using global modes based on high-fidelity simulation data. Optimal flow control was extracted from the model, and tested with high-fidelity simulation. ALCF computational scientists worked with the team to help optimize the parallel performance of the team's large-eddy simulation code.

RESULTS The team found that the new I/O modes contribute significantly to sound generation and explain the missing sound in the PSE analysis. This is significant because it is the first direct evidence that sideline noise can be explained in terms of coherent, non-compact acoustic sources rather than incoherent motions, as previously thought. These results have been published in the journal *Physics of Fluids*. High-fidelity simulations also precisely reproduced the dynamics of a laboratory supersonic jet striking a flat wall. Simulation data informed a reduced-order model that identified the key instability mechanism and provided a systematic way to control it. The team's simulations confirmed the effectiveness of the control (see figure), and suggested new laboratory experiments targeted at previously unknown physics.

IMPACT Guided by high-fidelity simulation, this approach could lead to a more universal acoustic source model than those commonly used in industry, and could become an important design tool. The systematic simulation and modeling methodology could revolutionize laboratory experiments by targeting them at otherwise undetected physics.



PREDICTIVE MODELING OF FUNCTIONAL NANOPOROUS MATERIALS

J. ILJA SIEPMANN
siepmann@umn.edu
University of Minnesota

ALCC

120 Million Core-Hours
Materials Science

Image: The reactive first-principles Monte Carlo (RxFPMC) approach to efficiently evaluate reaction equilibria was applied to compressed nitrogen-oxygen mixtures under conditions similar to atmospheric lightning strikes.

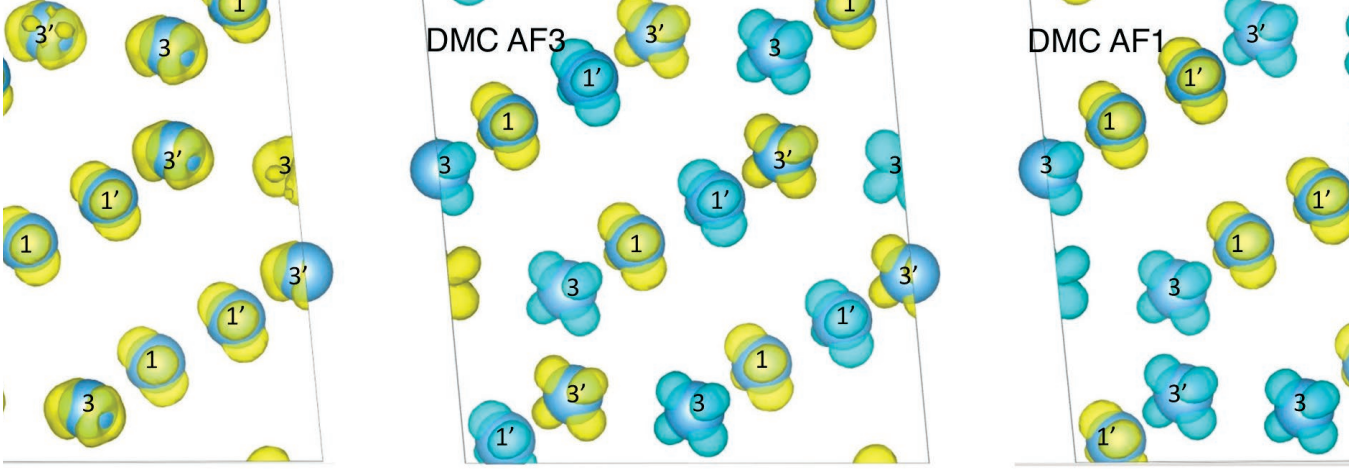
Image credit: Evgenii O. Fetisov and J. Ilja Siepmann, University of Minnesota

Nanoporous materials, such as metal-organic frameworks and zeolites, are of great interest to the biofuel and petrochemical industries because of their ability to act as sponges for gas storage, as molecular sieves for separations, and as catalysts that aid in the processing of fuels and chemical feedstocks. However, finding an optimal material for a given application is a time- and labor-intensive process that could take decades with traditional laboratory methods.

APPROACH Scientists participating in the DOE-funded Nanoporous Materials Genome Center, led by the University of Minnesota, are using Mira to demonstrate and develop a predictive theory and modeling tool that can rapidly screen thousands of materials to pinpoint promising candidates for further research. This research uses hierarchical screening workflows that involve machine learning, evolutionary algorithms, molecular simulations, and high-level electronic structure calculations. In addition, the team developed RxFPMC, a reactive first-principles Monte Carlo algorithm, to investigate reaction equilibria without the need for pre-specified chemical reactions and their ideal gas equilibrium constants. And with the petascale power of Mira, the screening workflows and RxFPMC algorithm can run all of the necessary replicas for different systems concurrently, significantly reducing the time to solution.

RESULTS In a paper published in *Angewandte Chemie*, the team used their screening workflows to find the 16 best all-silica zeolites for removing hydrogen sulfide from natural gas reserves. High levels of hydrogen sulfide "sour" reservoirs, making their exploration unprofitable. Using zeolites for removing hydrogen sulfide and "sweetening" the natural gas may be an economical solution for the sour natural gas problem. In another paper published in *ACS Central Science*, the researchers introduced the RxFPMC method and modeled highly compressed nitrogen-oxygen mixtures at the extreme conditions present in atmospheric lightning strikes and explosions. The team's RxFPMC method, which can overcome rare-event sampling problems, was validated by comparing the equilibrium distributions with those from the thermochemical Cheetah code parametrized to experimental data.

IMPACT With the ability to identify optimal zeolites and metal-organic frameworks for specific energy applications, this predictive modeling capability has the potential to benefit the production of biofuel and petroleum products, and the development of gas storage and carbon capture devices, while reducing the time and cost of associated research and development efforts.



QMC SIMULATIONS DATABASE FOR PREDICTIVE MODELING AND THEORY

DAVID CEPERLEY
ceperley@illinois.edu
University of Illinois at Urbana-Champaign

INCITE

170 Million Core-Hours (ALCF: 90M; OLCF: 80M)
Materials Science

Due to its numerical expense, quantum Monte Carlo (QMC) methods were once limited to model systems of small atoms or molecules. However, with supercomputers like Mira, QMC methods can be used for rigorous calculations on more complicated materials. This project is applying QMC on DOE leadership computing systems to improve predictive modeling of key properties found in energy-related or fundamental materials.

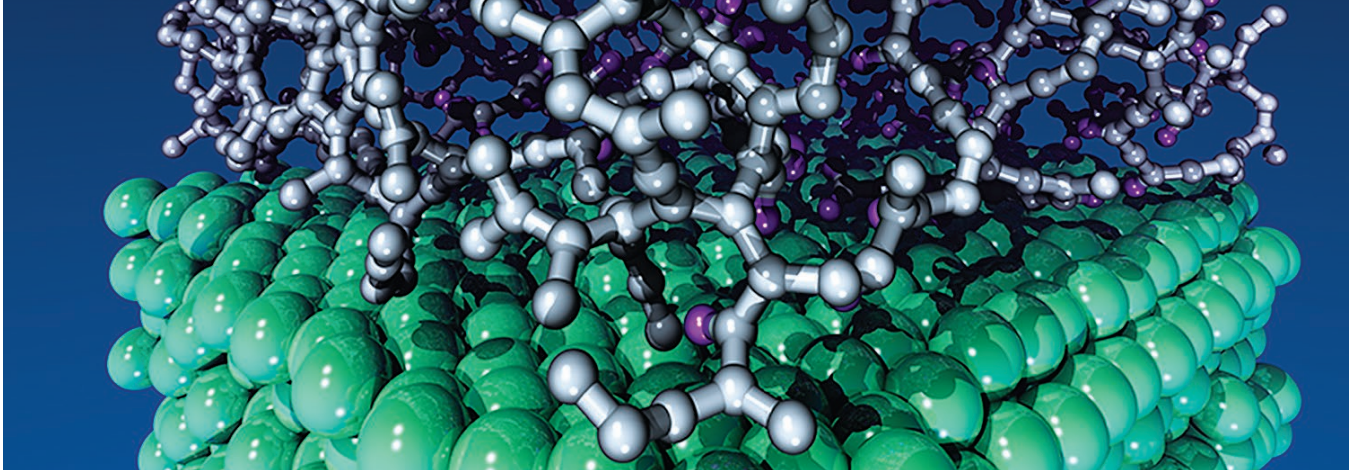
APPROACH Researchers are using the QMCPACK code for a variety of studies, including heterogeneous catalysis of transition metal nanoparticles, magnetic phase transitions, properties of materials under pressure, and strongly correlated materials showing interesting electronic and magnetic properties. ALCF computational scientists have improved the performance of QMCPACK by developing an interface between the fragmented molecular orbital method and QMC to increase the model system size up to 10,000 electrons with minimum loss of accuracy. By rewriting the code in IBM-specific language for Mira's architecture, they have also improved code performance by 30 percent.

RESULTS For one study, researchers modeled Ti_4O_7, a titanium oxide that has a range of technological applications due to its complex electronic and magnetic structures. Simulations on Mira have, for the first time, calculated the lowest energy states of Ti_4O_7, revealing its magnetic properties and stable ground state. The team's results were published in *Physical Chemistry Chemical Physics* and will help improve the accuracy of other electronic structure modeling tools, such as the widely used density functional theory. Additionally, researchers are studying the intermediate concentrations of iron-bearing perovskite and post-perovskite phases of magnesium silicate to better understand the unusual properties observed in the core-mantle boundary layer. Further, they are simulating platinum (Pt) solids, nanoclusters, and surfaces to analyze the surface energies of Pt (111) and Pt (100), which are important in surface and catalytic applications.

IMPACT This project aims to advance the efficiency and global applicability of QMC through the development of tools that make systematic research less time intensive. Its results are providing accurate predictions for energy-related materials and processes, such as transition metal oxides useful for electronics applications, perovskite phases of magnesium silicate found in the Earth's mantle, and platinum surfaces utilized in catalytic applications.

Image: Diffusion Monte Carlo spin densities for low-temperature Ti_4O_7 ferromagnetic (left), antiferromagnetic 3 (center), and antiferromagnetic 1 phases. Yellow represents a positive spin density (or spin up) and blue represents a negative spin density (or spin down).

Image credit: Anouar Benali and Olle Heinonen, Argonne National Laboratory



REACTIVE MD SIMULATIONS OF ELECTROCHEMICAL OXIDE INTERFACES AT MESOSCALE

SUBRAMANIAN SANKARANARAYANAN

skrssank@anl.gov
Argonne National Laboratory

INCITE

40 Million Core-Hours
Materials Science

The initial reactions important to chemical bond formation, electron transfer, and other electrochemical processes can occur on the atomistic and molecular scale in a matter of nanoseconds, beyond the detection of many experiments. For the design and development of new materials for energy applications, scientists need a fundamental understanding of these underlying processes that facilitate desirable electrochemical reactions, including resistance to corrosion and friction. In this project, researchers are simulating the reactive processes, including bond breakage and formation, at electrochemical interfaces on the order of millions of atoms.

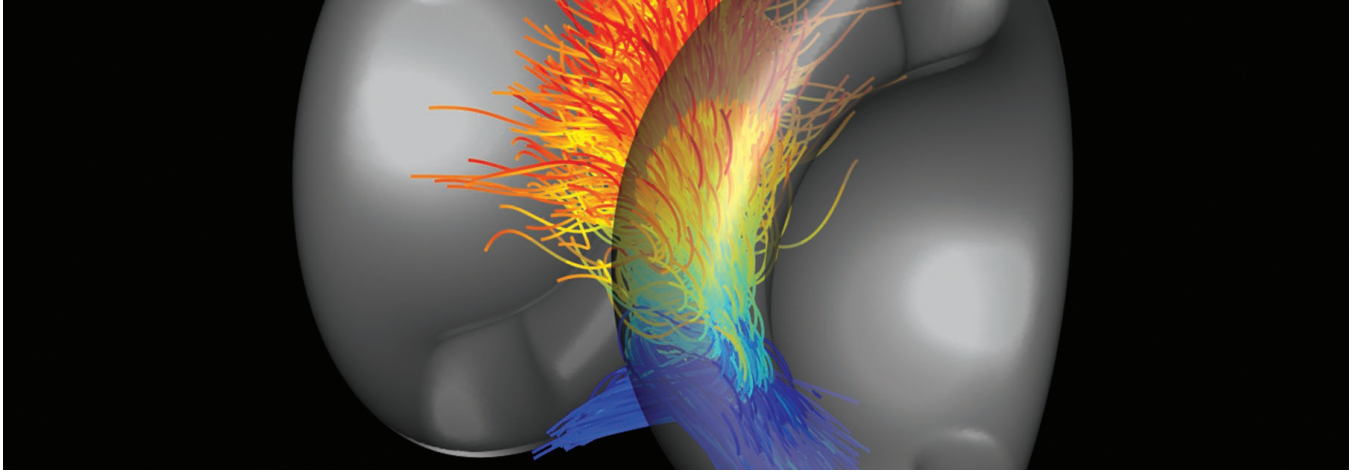
APPROACH Researchers from multiple computational and science domains at Argonne National Laboratory are simulating systems of over a million atoms on Mira using the LAMMPS molecular dynamics code with a ReaxFF module. ALCF staff assisted in doubling code performance by optimizing LAMMPS MPI communications on Mira's IBM Blue Gene/Q architecture and adding OpenMP threading to the ReaxFF module.

RESULTS After tribology experiments showed that a new film was being regenerated at the interface of an engine coating and base oil, researchers turned to Mira to model the underlying reactive processes. The simulations enabled the design of a self-healing, anti-wear coating that dramatically reduces friction and related degradation in engines and moving machinery. With LAMMPS, they modeled as many as two million atoms per simulation, making this one of the few atomistic studies of friction — of any kind, not just tribocatalysis — at this scale. Millions of time steps per simulation enabled researchers to identify the initial catalytic processes that occur within nanoseconds of machine operation. The results of the study were published in *Nature*. The researchers are now using their findings to virtually test other potential self-regenerating catalysts.

IMPACT Atomistic and molecular simulations are enabling researchers to understand the complex processes that make oils, coatings, electrodes, and other electrochemical interfaces effective. The computations are also allowing them to virtually test for new catalysts that may have useful properties.

Image: Visualization of a diamond-like carbon coating. Mira simulations have allowed an Argonne team to virtually test several potential catalysts (other metals and hydrocarbons in coatings and oils) for their self-healing properties in a high-temperature, high-pressure engine environment.

Image credit: Joseph A. Insley, Argonne National Laboratory



PARTICLE ACCELERATION IN SHOCKS: FROM ASTROPHYSICS TO LABORATORY IN SILICO

FREDERICO FIUZA

fiuza@slac.stanford.edu
SLAC National Accelerator Laboratory

INCITE

110 Million Core-Hours
Physics

Magnetic reconnection, a fundamental process in astrophysical and fusion plasmas in which magnetic energy is converted into plasma energy, is thought to lead to efficient particle acceleration. The process is critical for the evolution of a variety of systems, from astrophysics to nuclear fusion devices, and holds promise as a means of explaining particle acceleration in explosive cosmic phenomena.

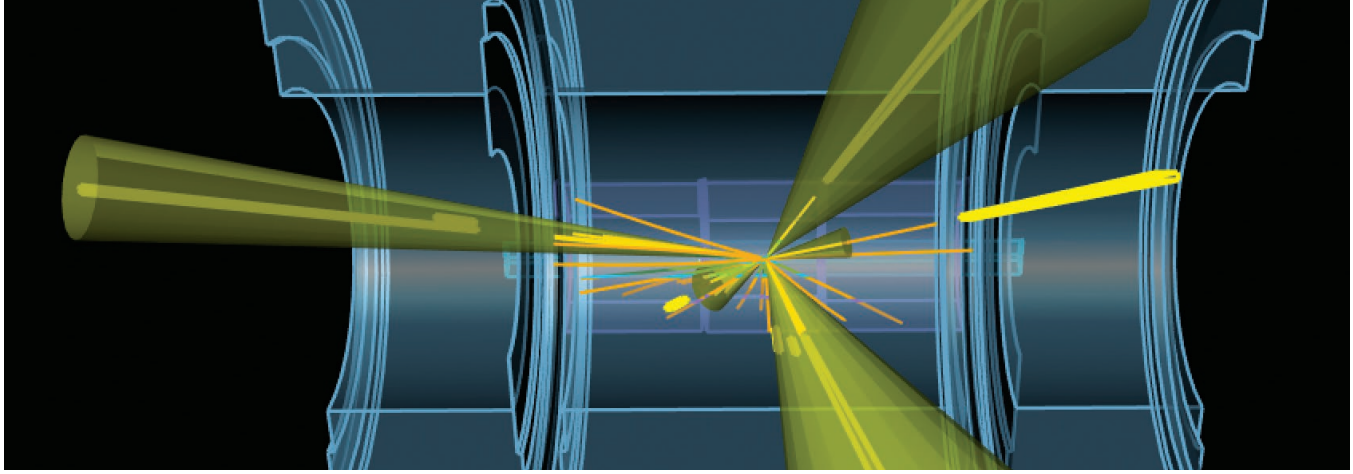
APPROACH Recent experiments studying laser-plasma interactions have shown the possibility of studying magnetic reconnection by using lasers to drive two plasma plumes that carry magnetic fields with opposite polarities. A laser blasts two foil targets, which are instantly turned into plasmas that expand and interact with each other. This INCITE project, an extension of similar work involving the development of particle acceleration in astrophysical shocks, is betting that these laboratory plasma experiments can shed light on the astrophysical processes that accelerate cosmic ray particles. Leveraging the relativistic massively parallel particle-in-cell (PIC) code OSIRIS, researchers conducted detailed simulations to study the possibility of observing particle acceleration in such an experimental setup — arguably the most important signature of reconnection. These were the first 3D simulations of laser-driven reconnection and the first to show the possibility of particle acceleration in this laboratory setting.

RESULTS The simulation results show that that laser-driven reconnection leads to strong non-thermal particle acceleration. As the two expanding plasma plumes interact with each other, they form a thin current sheet, or reconnection layer, which becomes unstable, breaking into smaller sheets. During this process, the magnetic field is annihilated and a strong electric field is excited in the reconnection region, strongly accelerating electrons as they enter the region. The accelerated electrons then escape in a fan-like profile, which leads to the development of a non-thermal particle distribution associated with some of the most explosive phenomena in the universe, such as solar flares and gamma ray bursts. The team's findings were published in *Physical Review Letters*.

IMPACT Results confirm that magnetic reconnection can lead to the efficient acceleration of astrophysical particles. The insight gained from these simulations may prove relevant not only to better understand the physics of cosmic rays, but also to design more efficient terrestrial accelerators for a variety of applications.

Image: A visualization from a 3D OSIRIS simulation of particle acceleration in laser-driven magnetic reconnection. The trajectories of the most energetic electrons (colored by energy) are shown as the two magnetized plasmas (grey isosurfaces) interact. Electrons are accelerated by the reconnection electric field at the interaction region and escape in a fan-like profile.

Image credit: Frederico Fiuza, SLAC National Accelerator Laboratory/ OSIRIS



PREDICTING THE TERASCALE ON-DEMAND WITH HIGH-PERFORMANCE COMPUTING

RADJA BOUGHEZAL
rboughezal@anl.gov
Argonne National Laboratory

Director's Discretionary

9 Million Core-Hours
Physics

Scientists analyzing data produced during the high-energy particle collisions at the Large Hadron Collider (LHC) are looking for subtle deviations from the Standard Model of particle physics. Using precision calculations, researchers can resolve discrepancies between theoretical predictions and experimental data. In the first run of the LHC, scientists discovered the Higgs boson. Now operating at a higher collision energy in its second run, researchers anticipate that even more exact calculations of particle interactions may address other outstanding problems in fundamental physics, including the nature of dark matter and the origin of matter-antimatter asymmetry.

APPROACH In this large-scale computational study, researchers from Argonne National Laboratory developed a novel framework adapted for supercomputers to perform precision calculations that are critical to advancing knowledge of phenomena such as dark matter. They used two-thirds of Mira's more than 49,000 nodes to predict the process of vector boson plus jet production, a particle interaction that is the dominant background in dark matter searches and has been measured by LHC experiments. The team's new framework maps the high-energy physics calculations to three separate many-dimensional integrals that are performed using importance-sampling Monte Carlo integration parallelized via MPI+OpenMP. Because this approach uses many sampling points to evaluate these integrals over the possible particle trajectories, Mira's massively parallel architecture is needed for unprecedented accuracy.

RESULTS The theoretical predictions produced on Mira explain an important class of measurements that had previously resisted theoretical explanation and will better enable researchers to track the rate of dark matter events in contrast to the barrage of similar events that take place in collisions. Results were published in a 2016 issue of *Physical Review Letters*.

IMPACT This project demonstrates that supercomputers can improve our ability to predict fundamental particle interactions in nature at the highest energies, making the most of experimental data and expediting searches for unknown particles and interactions.

With the theoretical framework developed at Argonne, researchers can more precisely predict particle interactions such as this simulation of a vector boson plus jet event.

Image credit: Taylor Childers, Argonne National Laboratory

EXPERTISE & RESOURCES

The ALCF's unique combination of supercomputing resources and expertise enables breakthroughs in science and engineering that would otherwise be impossible.

From left, ALCF staff members Amy Ying Li, David Martin, and Laura Ratcliff.

ALCF EXPERTISE

OUR PEOPLE SET US APART

The ALCF's talented and diverse staff make the facility one of the world's premier centers for computational science and engineering.

ALCF staff members gather in front of Argonne's Theory and Computing Sciences Building.

OPERATIONS

The Operations team is responsible for managing and supporting all ALCF computing systems, ensuring users have a stable, secure, and highly available resource to pursue their scientific goals. This includes overseeing the facility's supercomputers and computing clusters, network infrastructure, storage resources, and systems environments. In addition, the team develops and maintains a variety of tools that are critical to the seamless operation of the ALCF's supercomputing environment.

SCIENCE

The Science team works directly with ALCF users to maximize and accelerate their research efforts using the facility's computing resources. With multidisciplinary domain expertise, a deep knowledge of the ALCF computing environment, and experience with programming methods and community codes, the Science team helps users improve scientific productivity on ALCF computing resources and surmount any obstacles they may encounter along the way. The team is comprised of computational scientists, performance engineers, visualization experts, and data science experts.

USER EXPERIENCE

The User Experience team supports the ALCF user community by providing technical assistance, managing outreach and training, and stewarding stories about activities and research conducted at the facility. User Experience staff also lead the ALCF's efforts in industry outreach and business intelligence. The team's wide-ranging efforts include managing various user processes and interfaces, operating the help desk, facilitating user training events, developing facility stories, growing the base of industry users, and assimilating and verifying data to ensure accurate reporting of facility information.

2016 STATS

79

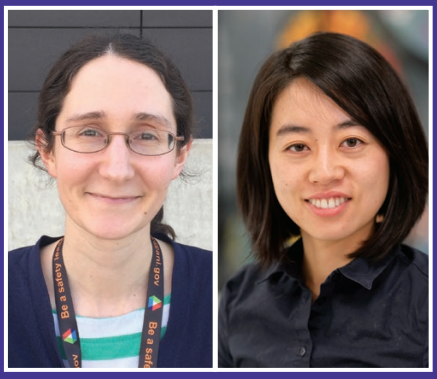
STAFF MEMBERS

15

POSTDOCTORAL RESEARCHERS

22

SUMMER STUDENTS



ALCF Announces its Next Margaret Butler Fellow

In June, the ALCF named Iowa State University graduate **Colleen Bertoni** as the next recipient of its Margaret Butler Fellowship in Computational Science. Bertoni, who was introduced at Argonne's annual Margaret Butler Celebration, will join the ALCF in 2017 to advance quantum chemistry studies of liquid water and ion solvation by employing and optimizing *ab initio*-based fragmentation methods on the facility's supercomputers.

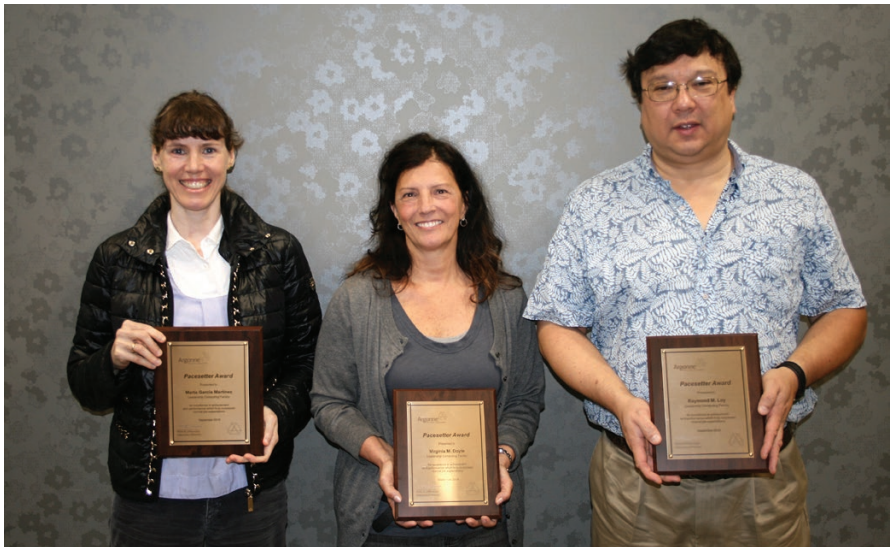
Bertoni will replace **Amy Ying Li**, the ALCF's first-ever Margaret Butler Fellow. A postdoctoral researcher from the University of Southern California, Li's two-year fellowship was focused on using ALCF supercomputers to study materials for advanced batteries. She is now continuing her work at the laboratory as an Argonne Research Scholar.

Two ALCF Staff Members Recognized by Argonne's Board of Governors

Susan Coghlan and Skip Reddy of the ALCF were recognized for their outstanding achievements to the laboratory at the 2016 University of Chicago, Argonne, LLC Board of Governors' awards ceremony in August.

Coghlan, who has served as the project director for all ALCF supercomputers, received the Distinguished Performance Award for her exceptional accomplishments in petascale computing technologies, advanced system software, and large-scale computational facilities — an area that Argonne has defined as one of its strategic initiatives and that the DOE has identified as critical to solving the nation's most important scientific and engineering problems.

Reddy, the ALCF's HPC Infrastructure Lead, was awarded the Excellence in Diversity and Inclusion Award for his founding and continued stewarding of Spectrum, an employee resource group for the lesbian, gay, bisexual, transgender, queer, and ally community at Argonne. As a result, he has helped promote a more welcoming and inclusive laboratory community.



Several Staff Members Honored with Pacesetter Awards

In 2016, 13 ALCF staff members received Argonne Pacesetter Awards, which are given to employees who have shown extraordinary initiative and dedication in their work at the laboratory.

Ben Allen was recognized for his role in making the Joint Laboratory for System Evaluation a critical resource for the laboratory, and for his efforts in support of the Theta Early Science Program.

Paul Coffman and William Scullin were recognized for their effort to bring the Joint Center for Energy Storage Research's Materials Project to production state on Mira.

Ginny Doyle was recognized for her contributions to the 2016 Argonne Training Program on Extreme-Scale Computing, including her support of the event website and other communications-related activities.

Marta Garcia and Ray Loy were recognized for their leadership in organizing and directing the 2016 Argonne Training Program on Extreme-Scale Computing.

Ye Luo was recognized for his work in implementing innovative technical improvements to advance the capabilities of the QMCPACK code.

Kevin Harms, Ed Holohan, Ryan Milner, Eric Pershey, Skip Reddy, and Paul Rich were recognized for their efforts and expertise leading up to and during the installation and acceptance of Theta.

ALCF Fills Two Leadership Positions

The ALCF filled two key leadership positions in 2016, with **Jini Ramprakash** hired as deputy division director and **Ti Leggett** coming aboard as the deputy project director/deputy director of operations.

In her new role, Ramprakash, who previously served as ALCF's user experience team lead, works closely with the ALCF director in planning, developing, implementing, and evaluating major initiatives of the division, including day-to-day operations and facility development.

Leggett comes to the ALCF from Argonne's Computing, Environment, and Life Sciences Directorate where he served as HPC systems administrator lead. In his role as deputy project director, Leggett assists the ALCF's project director in leading and managing large system deployment efforts, including Theta and Aurora. As deputy director of operations, he helps coordinate and manage the facility's operational activities.

STAFF SPOTLIGHTS

Anouar Benali

Computational Scientist

Anouar is one of the HPC community's foremost experts on the quantum Monte Carlo (QMC) approach, an important computational tool for performing accurate electronic structure calculations of atoms, molecules, and solids. As a developer of the QMCPACK simulation package, his work focuses on implementing and improving QMC algorithms for current supercomputers and future exascale systems. In 2016, Anouar began serving as co-principal investigator of a new Intel Parallel Computing Center, a collaborative effort aimed at optimizing QMCPACK for massively parallel computer systems based on the Intel® Many Integrated Core Architecture technology. He was also named co-principal investigator of an application development project involving QMPACK for DOE's new Exascale Computing Project. In addition, Anouar's recent work with an INCITE research team demonstrated the ability to use QMC simulations to accurately calculate the magnetic properties of a titanium oxide material for the first time. Their results were published in *Physical Chemistry Chemical Physics*.

Kevin Harms

Performance Engineer

From playing a lead role in the effort to deliver the facility's next-generation systems to working with users to optimize code performance, Kevin contributes to the ALCF mission in a multitude of ways. In 2016, he was a part of the team responsible for the successful acceptance of Theta. As the co-lead for the Aurora NRE (non-recurring engineering) effort, Kevin continues to work directly with Intel and Cray to resolve technical issues and to ensure all milestones are achieved. In the computational science realm, Kevin recently leveraged his I/O expertise to help an engine research team greatly improve the performance of the CONVERGE code on Mira. His optimization work enabled the team to carry out the largest engine simulation of its kind. Kevin is also a regular collaborator with the I/O research team in Argonne's Mathematics and Computer Science Division. Their work has included developing and deploying Darshan, a lightweight I/O instrumentation library, on ALCF systems to investigate the I/O behavior of production applications.

Janet Knowles

Software Developer

Prior to joining the ALCF's visualization team, Janet spent nearly a decade in the research and development industry working with mixed reality environments, 3D modeling, and real-time computer graphics. She is now leveraging that expertise to develop new ways for ALCF staff and users to interact with their projects. As her first order of business, Janet was charged with creating ALCF on the Move (OTM), a mobile productivity app that allows staff and users to access real-time information on ALCF resources anywhere at anytime. From collecting requirements and designing the user interface to writing the software front- and back-ends, Janet handled all aspects of developing ALCF OTM. Currently available to staff, the app provides information on ALCF system availability, running and scheduled jobs, and ALCF news and events. Janet is now preparing ALCF OTM for wider release so facility users can take advantage of the new tool as well. Also active in mentoring at the ALCF, Janet has worked with several undergraduate and graduate students on in-house visualization projects and libraries.

Ben Lenard

Database Administrator

Ben is responsible for overseeing the administration and improvement of database systems in the ALCF's supercomputing environment. These databases are critical to many of the facility's support services, including job scheduling, job accounting, and business intelligence. In 2016, Ben deployed the IBM Data Server Manager to help streamline database administration tasks. With this tool in place, Ben has a better idea of how the databases are being used, while developers have an improved method for identifying and addressing any performance issues with their queries. Ben gave a presentation on his experience with the tool at the 2016 IBM World of Watson conference in Las Vegas. In addition to his day-to-day responsibilities, Ben has been a strong advocate for the ALCF and for computer science, volunteering for events like the Hour of Code and Argonne's public open house. He is also currently pursuing a PhD in Computer and Information Sciences at DePaul University.

Preeti Malakar

Postdoctoral Researcher

For her doctoral studies at the Indian Institute of Science, Bangalore, Preeti worked on efficient high-fidelity weather simulations, online data analysis, and remote visualization in resource-constrained computational environments. As a postdoctoral researcher with the ALCF's visualization team, she is now building off of her previous work to develop novel computational methods for some of the world's most powerful computing resources. Preeti's work includes developing *in situ* analysis techniques for large-scale molecular dynamics and astrophysics simulations, devising solutions to execute optimal simulation-analysis workflows, and improving I/O performance through better routing of data flows. In 2016, she co-authored a paper in the journal *Parallel Computing* that details a new algorithm designed to improve I/O performance on Mira. By routing data to the closest I/O nodes and reducing network congestion, the algorithm successfully reduced write times by an average of 60 percent over the default independent I/O.

Doug Waldron

Data Architect

In a Star Trek Borg-themed talk to ALCF staff earlier this year, Doug explained that the ultimate goal of his business intelligence team is "achieving data perfection." Since joining the ALCF in 2013, Doug has become the facility's go-to guy for all data-related inquires, which can range from machine utilization graphs to information about the ALCF user community. As an example, Doug's team is responsible for providing data for the ALCF's annual Operational Assessment Report, which calls for 63 metrics, 23 graphs, and 12 reports. Under his leadership, the small, but productive business intelligence team has developed automated tools to assimilate and perfect erratic and conflicted data from several different systems at the facility. In 2016, Doug led the expansion of the ALCF's Data Warehouse to include data from Theta, Darshan, Tracklib, and Autoperf. All in all, his business intelligence efforts have helped to eliminate the burden of data collection, maintenance, analysis, and reporting from several other groups at the ALCF.

ALCF-DEVELOPED SOFTWARE TOOLS

ALCF researchers are developing software tools and approaches to help scientific applications run more efficiently on its leadership-class systems, and to provide valuable information to guide future support and research priorities.

AutoPerf

AutoPerf is an ALCF-developed library that automatically collects performance information for applications running on ALCF systems. The tool records data from simulations and saves it for analysis when the job is completed. Output includes MPI usage and performance information that indicates which MPI routines were called, how many times each routine was called, the time spent in each routine, the number of bytes sent or received (if applicable), and data from the system's hardware performance counters. This information is helping ALCF staff better understand the requirements of applications and how to optimize their performance.

Business Intelligence Tools

The ALCF's Business Intelligence (BI) team is responsible for assimilating and verifying data from many ALCF systems to ensure the accurate reporting of facility information to users, ALCF leadership, and DOE. This includes producing everything from real-time usage graphs to facility data for quarterly and yearly reports. The BI team has developed automated systems to continuously extract the data from several disjointed systems at the facility and convert the data into dimension and fact tables with a standard set of units. The data is loaded into a centralized database known as the Data Warehouse. Additional processing combines multiple datasets into smaller datasets suitable for use by the BI team's reporting software. The team has automated tools in place to ensure the accuracy and completeness of all data pulled from the Data Warehouse. BI also maintains Pentaho, an ad hoc reporting system that allows ALCF staff members to execute complex queries and visualize resulting datasets. These efforts have greatly improved the efficiency of data collection, maintenance, analysis, and reporting at the ALCF.

Cobalt

Developed at Argonne, Cobalt is the ALCF's job scheduler and resource manager. This tool gives the facility great flexibility in executing its scheduling policies, accommodates diverse workloads, and provides important features (e.g., alternate kernel support) that are either not supported or poorly supported by other schedulers and resource managers. In 2016, the ALCF continued work to prepare Cobalt for its next-generation systems. The tool now has the ability to interface with and run on Cray systems, starting with the XC40 platform, significantly broadening the types of systems on which Cobalt can be installed. This functionality enabled ALCF researchers to use Cobalt to drive the successful acceptance testing of Theta. In addition, Cobalt's data-staging capabilities were enhanced to allow users to stage specific files to ALCF storage from external facilities, such as Argonne's Advanced Photon Source, using Globus Online to broker the transfer in a secure manner. This Cobalt improvement is also a critical first step to adding more data-centric features, such as handling non-volatile node-local storage and burst-buffer capabilities, in preparation for Aurora.

Compiler and Library Tracking

The ALCF has developed and deployed two software tools — Trackdeps and Tracklib — to track the compilers and libraries being used on its systems. The first stage in the library-tracking process is Trackdeps, which records paths to all build process inputs that contribute to the final output, including compiler identity, header files, Fortran module files, and libraries. Tracklib, the second stage in the library-tracking process, is a set of tools used to examine programs as they run on Mira, producing the data necessary to match the job's accounting information with the data collected by Trackdeps. With these tools in place, staff can determine how various libraries and compilers are being used at the facility, providing knowledge that helps inform support and ALCF and DOE research priorities.

A web-based tool called the Gronkulator pulls machine status information from Colbalt to provide users and staff with a real-time look at ALCF system activity.

Darshan

ALCF researchers are collaborating with staff from Argonne's Mathematics and Computer Science Division on the continued development of Darshan, a scalable HPC I/O instrumentation library designed to capture an accurate picture of application I/O behavior. This tool records statistics such as the number of files opened, time spent performing I/O, and the amount of data accessed by an application. Darshan's lightweight design makes it suitable for full-time deployment for workload characterization of large systems. The information revealed by Darshan enables researchers to investigate and tune the I/O behavior of complex HPC applications, while also helping the storage research community to develop strategies and approaches to better serve the needs of scientific computing. Darshan is portable across a wide variety of platforms and is now deployed at multiple DOE computing facilities. In 2016, the development team released a new modularized version of Darshan (version 3).

Job Failure Analysis

Every week, the ALCF Operations team analyzes all job failures that occur at the facility to resolve any system-related issues and to identify issues that could help improve user productivity. To help with this analysis, the ALCF has developed a system to allow interactive querying of job data and annotation of job status. This system helps ALCF staff determine the fate of every job with a non-zero exit code. Instead of many people talking to the one person who has specific job information, the system allows staff to save the data in a database in real time. The system has also eliminated much of the manual log parsing that individuals were doing to find out what really happened to a particular job. In 2016, ALCF staff began adapting the job failure analysis software for its next-generation systems, Theta and Aurora, as part of the development of the Operational Data Processing Service (ODPS). In addition to being the core of the job failure analysis data, ODPS tracks usage, availability, reservations, jobs, or any event that happens over time using an ALCF computing resource.

sbank

In December, the ALCF deployed sbank, a new job accounting system that will replace the facility's original accounting tool, cbank. The customized software system, which processes output from the Cobalt scheduler, is designed to allow users to track project allocations, usage charges, and refunds. It gives users the ability to query the balance and expiration of their project, and enables them to manage and monitor their allocation usage by user, job, and computing system. The new sbank software has similar syntax to cbank, but provides enhanced options for displaying allocation information, giving users much more flexibility in how they can query and report usage data.

ALCF COMPUTING RESOURCES

THETA

Theta, a 9.65-petaflops supercomputer, serves as a bridge between Mira and the ALCF's next leadership-class system, Aurora. Theta will be used for computational science and engineering research, while providing an early production system to help ALCF users transition their applications to the new Cray/Intel® Xeon Phi™ architecture.

- Cray/Intel® Xeon Phi™ architecture
- 9.65 petaflops
- 64-core 1.3 GHz Intel 7230 processor per node
- 3,624 nodes
- 231,935 cores
- 679 TB of memory
- 56 TB of high-bandwidth memory
- Aries interconnect with Dragonfly configuration
- 20 racks

MIRA

Mira is the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer. In addition to being one of the most powerful supercomputers in the world, Mira is also among the most energy efficient. The system saves considerable energy through innovative chip designs and a unique water-cooling system.

- IBM Blue Gene/Q architecture
- 10 petaflops
- 16-core 1.6 GHz IBM PowerPC A2 processor per node
- 49,152 nodes
- 786,432 cores
- 768 TB of memory
- 5D torus interconnect
- 48 racks

COOLEY

Cooley is the ALCF's data analysis and visualization cluster. The system helps researchers analyze and explore the massive datasets that result from their simulations on Mira. Cooley shares file systems with the supercomputer, enabling direct access to Mira-generated results.

- Intel® Haswell architecture
- 293 teraflops
- 2 6-core 2.4 GHz Intel E5-2620 processors per node
- 1 NVIDIA Tesla K80 GPU per node
- 126 nodes
- 1,512 cores
- 47 TB of memory
- 3 TB of GPU memory
- FDR Infiniband interconnect
- 6 racks

CETUS

Cetus is an IBM Blue Gene/Q system used to offload both debugging issues and alternative production workloads from Mira. To facilitate these activities, Cetus shares the same software environment and file systems as Mira.

- IBM Blue Gene/Q architecture
- 838 teraflops
- 16-core 1.6 GHz IBM PowerPC A2 processor per node
- 4,096 nodes
- 65,536 cores
- 64 TB of memory
- 5D torus interconnect
- 4 racks

VESTA

Vesta, an IBM Blue Gene/Q system, serves at the ALCF's test and development platform, providing a computing resource for researchers preparing to use Mira.

- IBM Blue Gene/Q architecture
- 419 teraflops
- 16-core 1.6 GHz IBM PowerPC A2 processor per node
- 2,048 nodes
- 32,768 cores
- 32 TB of memory
- 5D torus interconnect
- 2 racks

DATA STORAGE

At the ALCF, disk storage provides intermediate-term storage for active projects, offering a means to access, analyze, and share simulation results. Tape storage is used to archive data from completed projects.

DISK STORAGE The Blue Gene/Q data systems consist of 384 I/O nodes that connect to 22 storage arrays that control 13,000 disk drives with a total useable capacity of 27 PB and a maximum aggregate transfer speed of 330 GB/s over two file systems. The ALCF uses the General Parallel File System to access the storage.

TAPE STORAGE The ALCF has three 10,000-slot libraries using LTO 6 tape technology. The LTO tape drives have built-in hardware compression with compression ratios typically between 1.25:1 and 2:1, depending on the data, giving an effective capacity of 36-60 PB.

NETWORKING

The Blue Gene/Q systems have an internal proprietary network for communicating between nodes. InfiniBand enables communication between the I/O nodes and the storage system. Ethernet is used for external user access, and for maintenance and management of the systems.

The ALCF connects to other research institutions using up to 100 Gb/s of network connectivity. Scientists can transfer datasets to and from other institutions over fast research networks, such as the Energy Science Network (ESNet) and Internet2.

APPENDIX I: ALCF PUBLICATIONS

Researchers who use 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.

In 2016, research at the ALCF resulted in more than 250 publications. The following list is ordered by publication month. An asterisk after a name indicates an ALCF author. ALCF publications are listed online at: alcf.anl.gov/publications.

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APPENDIX II: ALCF PROJECTS

2016 INCITE PROJECTS

BIOLOGICAL SCIENCES

Multiscale Simulations of Human Pathologies
George Karniadakis, Brown University
90 Million Core-Hours (ALCF: 50M; OLCF: 40M)

Protein-Protein Binding Specificity
Benoît Roux, The University of Chicago/Argonne National Laboratory
160 Million Core-Hours

CHEMISTRY

Evaluation of a 1000 MW Commercial Ultra Super-Critical Coal Boiler
Martin Berzins, University of Utah
351 Million Core-Hours (ALCF: 280M; OLCF: 71M)

First-Principles Simulations of High-Speed Combustion and Detonation
Alexei Khokhlov, The University of Chicago
140 Million Core-Hours

Towards Breakthroughs in Protein Structure Calculation and Design
David Baker, University of Washington
120 Million Core-Hours

COMPUTER SCIENCE

Dynamic and Adaptive Parallel Programming for Exascale Research
Robert Harrison, Stony Brook University
20 Million Core-Hours

Performance Evaluation and Analysis Consortium (PEAC) End Station
Leonid Oliker, Lawrence Berkeley National Laboratory
90 Million Core-Hours (ALCF: 45M; OLCF: 45M)

EARTH SCIENCE

Accelerated Climate Modeling for Energy
Mark Taylor, Sandia National Laboratories
180 Million Core-Hours (ALCF: 100M; OLCF: 80M)

Frontiers in Planetary and Stellar Magnetism Through High-Performance Computing
Jonathan Aurnou, University of California, Los Angeles
150 Million Core-Hours

High-Frequency Ground Motion Simulation for Seismic Hazard Analysis
Thomas Jordan, University of Southern California
190 Million Core-Hours (ALCF: 90M; OLCF: 100M)

ENGINEERING

Adaptive Detached-Eddy Simulation of a High Lift Wing with Active Flow Control
Kenneth Jansen, University of Colorado Boulder
50 Million Core-Hours

Convective Turbulence in Liquid Gallium and Sodium
Janet Scheel, Occidental College
80 Million Core-Hours

Direct Numerical Simulation of Compressible, Turbulent Flow
Jonathan Poggie, Purdue University
150 Million Core-Hours

Direct Numerical Simulations and Robust Predictions of Cloud Cavitation Collapse
Petros Koumoutsakos, ETH Zürich
72 Million Core-Hours

Large-Eddy Simulations of Combustor Liner Flows
Anne Dord, GE Aviation
100 Million Core-Hours

MATERIALS SCIENCE

Charge Transport in Thin Film Ionomers
Gregory Voth, The University of Chicago
100 Million Core-Hours

Combining High-Accuracy Electronic Structure Methods to Study Surface Reactions
Maria Chan, Argonne National Laboratory
50 Million Core-Hours

Computational Spectroscopy of Heterogeneous Interfaces
Giulia Galli, The University of Chicago/Argonne National Laboratory
François Gygi, University of California, Davis
150 Million Core-Hours

Electronic Response to Particle Radiation in Condensed Matter
André Schleife, University of Illinois at Urbana-Champaign
70 Million Core-Hours

Petascale Simulations of Self-Healing Nanomaterials
Rajiv Kalia, University of Southern California
180 Million Core-Hours

QMC Simulations Database for Predictive Modeling and Theory
David Ceperley, University of Illinois at Urbana-Champaign
170 Million Core-Hours (ALCF: 90M; OLCF: 80M)

Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale
Subramanian Sankaranarayanan, Argonne National Laboratory
40 Million Core-Hours

SiO2 Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme
James Kermode, University of Warwick
126 Million Core-Hours

ALCF PROJECTS CONTINUED

State-of-the-Art Simulations of Liquid Phenomena
Mark Gordon, Iowa State University
200 Million Core-Hours

Unveiling the Behavior of UO2 Under Extreme Physical Conditions
Peter Littlewood, Argonne National Laboratory
75 Million Core-Hours

PHYSICS

Cosmic Reionization on Computers
Nickolay Gnedin, Fermilab
65 Million Core-Hours

Cosmological Simulations for Large-Scale Sky Surveys
Salman Habib, Argonne National Laboratory
150 Million Core-Hours (ALCF: 80M; OLCF: 70M)

Fundamental Properties of QCD Matter Produced at RHIC and the LHC
Claudia Ratti, University of Houston
100 Million Core-Hours

Kinetic Simulations of Relativistic Radiative Magnetic Reconnection
Dmitri Uzdensky, University of Colorado Boulder
90 Million Core-Hours

Lattice QCD
Paul Mackenzie, Fermilab
280 Million Core-Hours (ALCF: 180M; OLCF: 100M)

Magnetohydrodynamic Models of Accretion, Including Radiation Transport
James Stone, Princeton University
47 Million Core-Hours

Nuclear Structure and Nuclear Reactions
James Vary, Iowa State University
184 Million Core-Hours (ALCF: 80M; OLCF: 104M)

Petascale Simulation of Magnetorotational Core-Collapse Supernovae
Sean Couch, Michigan State University
100 Million Core-Hours

Petascale Simulations of Laser Plasma Interaction Relevant to IFE
Frank Tsung, University of California, Los Angeles
100 Million Core-Hours

2015-2016 ALCC PROJECTS

CHEMISTRY

Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral Ab Initio Study
Robert A. DiStasio, Cornell University
175 Million Core-Hours

Computational Design of Interfaces for Photovoltaics
Noa Marom, Tulane University
120 Million Core-Hours (ALCF: 100M; NERSC: 20M)

PT-Symmetric Quantum Mechanics for Real-Time Electron Transport Simulations
Hanning Chen, George Washington University
16 Million Core-Hours

COMPUTER SCIENCE

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications
Robert Voigt, Leidos Inc.
167 Million Core-Hours
(ALCF: 127M; OLCF: 40M)

Performance Analysis, Modeling, and Scaling of HPC Applications and Tools
Abhinav Bhatele, Lawrence Livermore National Laboratory
29.4 Million Core-Hours (ALCF: 20.1M; OLCF: 9.3M)

Portable Application Development for Next-Generation Supercomputer Architectures
Tjerk Straatsma, Oak Ridge National Laboratory
160 Million Core-Hours (ALCF: 60M; NERSC: 40M; OLCF: 60M)

EARTH SCIENCE

Delivering the Department of Energy's Next-Generation High-Resolution Earth System Model
Peter Thornton, Oak Ridge National Laboratory
165 Million Core-Hours (ALCF: 110M; OLCF: 55M)

Validation of RAP/HRRR for the Wind Forecast Improvement Project II
Joe Olson, National Oceanic and Atmospheric Administration
15 Million Core-Hours

ENGINEERING

Advancing Internal Combustion Engine Simulations Using Sensitivity Analysis
Sibendu Som, Argonne National Laboratory
60 Million Core-Hours

Computational Design of Novel Multiscale Concrete Rheometers
William George, National Institute of Standards and Technology
50 Million Core-Hours

Credible Predictive Simulation Capabilities for Advanced Clean Energy Technology Development Through Uncertainty Quantification
Aytekin Gel, ALPEMI
111.5 Million Core-Hours

High-Fidelity Computations of Fuel Assemblies Subjected to Seismic Loads
Elias Balaras, George Washington University
34 Million Core-Hours

Large-Eddy Simulation of Turbine Internal Cooling Passages
Gustavo Ledezma, GE Global Research
6 Million Core-Hours

Toward a Longer-Life Core: Thermal-Hydraulic CFD Simulations of Deformed Fuel Assemblies
Elia Merzari, Argonne National Laboratory
72 Million Core-Hours

MATERIALS SCIENCE

First-Principles Large-Scale Simulations of Interfaces for Energy Conversion and Storage
Marco Govoni, The University of Chicago/Argonne National Laboratory
75 Million Core-Hours

Large-Scale Ab Initio Simulation of Crystalline Defects in Mg-Alloys
Kaushik Bhattacharya, Caltech
20 Million Core-Hours

Predictive Modeling of Functional Nanoporous Materials
J. Ilja Siepmann, University of Minnesota
120 Million Core-Hours

Revealing the Reversible Electrodeposition Mechanism in Multivalent-Ion Batteries
Gerbrand Ceder, Massachusetts Institute of Technology
70 Million Core-Hours

PHYSICS

Cosmic Frontier Computational End-Station
Salman Habib, Argonne National Laboratory
115 Million Core-Hours (ALCF: 65M; NERSC: 15M; OLCF: 35M)

An End-Station for Intensity and Energy Frontier Experiments and Calculations
Thomas LeCompte, Argonne National Laboratory
78 Million Core-Hours (ALCF: 62M; NERSC: 16M)

Extreme-Scale Particle Simulation to Carry Out the 2016 FES National Theory and Simulation Performance Target
Choong-Seock Chang, Princeton Plasma Physics Laboratory
10 Million Core-Hours

Hadronic Light-By-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions
Thomas Blum, University of Connecticut
175 Million Core-Hours

Large-Eddy Simulation and Direct Numerical Simulation of Fluid Induced Loads on Reactor Vessel Internals
Milorad Dzodzo, Westinghouse
40 Million Core-Hours

Numerical Simulation of Turbulent Flows in Advanced Steam Generators
Aleksandr Obabko, Argonne National Laboratory
25.4 Million Core-Hours

Understanding Helium-Hydrogen Plasma Mediated Tungsten Surface Response to Predict Fusion Plasma-Facing Component Performance in ITER
Brian Wirth, University of Tennessee
116 Million Core-Hours (ALCF: 80M; OLCF: 36M)

Validation Simulations of Macroscopic Burning-Plasma Dynamics
Jacob King, Tech-X
40 Million Core-Hours

2016-2017 ALCC PROJECTS

BIOLOGICAL SCIENCES

Molecular Dynamics Studies of Biomass Degradation in Biofuel Production
Emad Tajkhorshid, University of Illinois at Urbana-Champaign
50 Million Core-Hours

CHEMISTRY

Molecular Modeling of Hot Electron Transfer for Solar Energy Conversion
Hanning Chen, George Washington University
16 Million Core-Hours

COMPUTER SCIENCE

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications
Robert Voigt, Leidos Inc.
191 Million Core-Hours (ALCF: 151M; OLCF: 40M)

EARTH SCIENCE

Delivering the Department of Energy's Next-Generation High-Resolution Earth System Model
Peter Thornton, Oak Ridge National Laboratory
211 Million Core-Hours (ALCF: 158M; OLCF: 53M)

ENGINEERING

Adjoint-Based Optimization via Large-Eddy Simulation of a Fundamental Turbine Stator-Rotor
Qiqi Wang, Massachusetts Institute of Technology
15 Million Core-Hours

Computational Study of Cycle-to-Cycle Variation in Dual-Fuel Engines
Ravichandra Jupudi, GE Global Research
25 Million Core-Hours

Credible Predictive Simulation Capabilities for Advanced Clean Energy Technology Development through Uncertainty Quantification
Aytekin Gel, ALPEMI
17 Million Core-Hours

Multiphase Simulations of Nuclear Reactor Flows
Igor Bolotnov, North Carolina State University
72.1 Million Core-Hours

Unraveling Silent Owl Flight to Develop Ultra-Quiet Energy Conversion Machines
Anupam Sharma, Iowa State University
25 Million Core-Hours

MATERIALS SCIENCE

Computational Engineering of Defects in Soft and Hard Materials for Energy and Quantum Information Applications
Marco Govoni, The University of Chicago/Argonne National Laboratory
53.7 Million Core-Hours

First-Principles Design and Analysis of Energy-Efficient NanoElectronic Switches
Sefa Dag, Globalfoundries
10 Million Core-Hours

First-Principles Design of Magnetic Materials, Models, and Mechanisms
Lucas Wagner, University of Illinois at Urbana-Champaign
30 Million Core-Hours

Modeling Helium-Hydrogen Plasma Mediated Tungsten Surface Response to Predict Fusion Plasma-Facing Component Performance in ITER
Brian Wirth, University of Tennessee
95 Million Core-Hours (ALCF: 70M; OLCF: 25M)

Modeling of Intense X-Ray Laser Dynamics in Nanoclusters
Phay Ho, Argonne National Laboratory
10 Million Core-Hours

Predictive Modeling of Functional Nanoporous Materials, Nanoparticle Assembly, and Reactive Systems
J. Ilja Siepmann, University of Minnesota
117 Million Core-Hours

The Materials Project: Completing the Space of Elastic and Piezoelectric Tensors
Kristin Persson, Lawrence Berkeley National Laboratory
36 Million Core-Hours

PHYSICS

61-Pin Wire-Wrap Turbulent Conjugate-Heat Transfer: V&V for Industry and SESAME
Elia Merzari, Argonne National Laboratory
120 Million Core-Hours

Ab Initio Modeling of the Dynamical Stability of HED Plasmas: From Fusion to Astrophysics
Frederico Fiuza, SLAC National Accelerator Laboratory
60 Million Core-Hours

An End-Station for Intensity and Energy Frontier Experiments and Calculations
Taylor Childers, Argonne National Laboratory
106.5 Million Core-Hours (ALCF: 93.5M; NERSC: 13M)

Exploring Higgs Compositeness Mechanism in the Era of the 14 TeV LHC
George Fleming, Yale University
55 Million Core-Hours

Extreme-Scale Gyrokinetic Particle Simulations to Complete the 2016 OFES National Theory/Simulation Performance Target and to Study the Fundamental Edge Physics
Choong-Seock Chang, Princeton Plasma Physics Laboratory
175 Million Core-Hours (ALCF: 100M; OLCF: 75M)

Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions
Thomas Blum, University of Connecticut
180 Million Core-Hours

High-Intensity Multibunch Physics in the Fermilab Accelerator Complex
James Amundson, Fermilab
50 Million Core-Hours

Muon g–2 Hadronic Vacuum Polarization from Lattice QCD
John Laiho, Syracuse University
66 Million Core-Hours

Nuclear Structure for Tests of Fundamental Symmetries and Astroparticle Physics
Calvin Johnson, San Diego State University
30 Million Core-Hours (ALCF: 6M; NERSC: 24M)

Numerical Simulation of Turbulent Flows in Advanced Steam Generators
Aleksandr Obabko, Argonne National Laboratory
80 Million Core-Hours

Simulations of Laser Experiments to Study the Origin of Cosmic Magnetic Fields
Petros Tzeferacos, The University of Chicago
60 Million Core-Hours

2016 DIRECTOR'S DISCRETIONARY PROJECTS

The following list provides a sampling of the many Director's Discretionary projects at the ALCF.

BIOLOGICAL SCIENCES

Computing 3D Structures of RNA from Small-Angle X-Ray Scattering Data and Secondary Structures
Yuba Bhandari and Yun-Xing Wang, National Cancer Institute
15 Million Core-Hours

CHEMISTY

First-Principles Monte Carlo Algorithm Development and Implementation in CP2K
Neeraj Rai, Mississippi State University
1.5 Million Core-Hours

First-Principles Simulation of Electronic Excitation Dynamics in Liquid Water and DNA Under Proton Irradiation
Yosuke Kanai, University of North Carolina
3 Million Core-Hours

Folding and Stability of an Intrinsically Disordered Domain in Estrogen Receptor
Sichun Yang, Case Western Reserve University
9.5 Million Core-Hours

Modeling Nonadiabatic Spin-Forbidden Reaction Mechanisms in Metal-Sulfur Proteins
Sergey Varganov, University of Nevada, Reno
1.5 Million Core-Hours

QuanPol QMMM-Style MP2 Simulation Methods
Hui Li, The University of Chicago
1 Million Core-Hours

Scaling of the FMO Method for Heterogeneous Systems
Casper Steinmann Svendsen, University of Bristol
2.4 Million Core-Hours

COMPUTER SCIENCE

HPC Applications Tuning
Khaled Ibrahim, Lawrence Berkeley National Laboratory
4 Million Core-Hours

Interfacial Behavior of Alcohol at Water/Organic Biphasic System
Baofu Qiao, Argonne National Laboratory
1.2 Million Core-Hours

Nek Performance Evalutation
Oana Marin, Argonne National Laboratory
1 Million Core-Hours

Scalable Analysis Methods and In Situ Infrastructure for Extreme-Scale Knowledge Discovery
Venkat Vishwanath, Argonne National Laboratory
2.4 Million Core-Hours

SciDAC Scalable Data Management Analysis and Visualization
Joseph A. Insley and Michael E. Papka, Argonne National Laboratory
2.5 Million Core-Hours

EARTH SCIENCE

Contrail-Cirrus Sensitivity to Turbulence Fluctuations Using LES Data
Roberto Paoli, University of Illinois at Chicago
1 Million Core-Hours

ENGINEERING

Computational Modeling of the Human Eye
Marco L. Bittencourt, University of Campinas
5 Million Core-Hours

Direct Numerical Simulation of Bachalo-Johnson Transonic Separated Flow
Philippe Spalart, Boeing
5.9 Million Core-Hours

High-Fidelity Simulations of Complex Turbulent Flows
Krishnan Mahesh, University of Minnesota
3.9 Million Core-Hours

Influence of Duct Corner Geometry on Secondary Flow: Convergence from Duct to Pipe Flow
Hassan M. Nagib, Illinois Institute of Technology
2.4 Million Core-Hours

Multiphase Simulations of Nuclear Reactor Thermal Hydraulics
Igor A. Bolotnov, North Carolina State University
7.6 Million Core-Hours

New Pathways to Stability and Instability in Rayleigh-Taylor Non-Premixed Flames
Praveen Ramaprabhu, University of North Carolina at Charlotte
1.9 Million Core-Hours

Variable-Density Fluid Dynamics
Paul E. Dimotakis, California Institute of Technology
2.2 Million Core-Hours

MATERIALS SCIENCE

Ion Transport in Li-S Solid
Ying Li, Argonne National Laboratory
7. 4 Million Core-Hours

Integrating Simulation and Observation: Discovery Engines for Big Data
Rajkumar Kettimuthu and Justin M. Wozniak, Argonne National Laboratory
6 Million Core-Hours

PHYSICS

Beam Dynamics Simulations for the Advanced Photon Source Upgrade
Michael Borland, Argonne National Laboratory
12.5 Million Core-Hours

NEAMS Neutronics Verification and Validation Simulations
Emily Shemon, Argonne National Laboratory
5.5 Million Core-Hours

Quantum Monte Carlo for Spin-Orbit Interactions, Spintronic and Van Der Waals Systems
Lubos Mitas, North Carolina State University
2.3 Million Core-Hours

Particle-In-Cell Scalable Spectral Relativistic
Jean-Luc Vay, Lawrence Berkeley National Laboratory
1.1 Million Core-Hours

Predicting the Terascale On-Demand with High-Performance Computing
Radja Boughezal, Argonne National Laboratory
9 Million Core-Hours

Using Quantum Monte Carlo for Magnetic Materials
Lucas K. Wagner, University of Illinois at Urbana-Champaign
8 Million Core-Hours

White Dwarf Mergers on Adaptive Meshes
Maximilian Katz, Stony Brook University
2.7 Million Core-Hours

About Argonne Leadership Computing Facility

Argonne's Leadership Computing Facility Division operates the Argonne Leadership Computing Facility as part of the U.S. Department of Energy's effort to provide leadership-class computing resources to the scientific community. The ALCF is supported by the DOE Office of Science, Advanced Scientific Computing Research (ASCR) program.

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Argonne NATIONAL LABORATORY

CONTACT
media@alcf.anl.gov
alcf.anl.gov

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