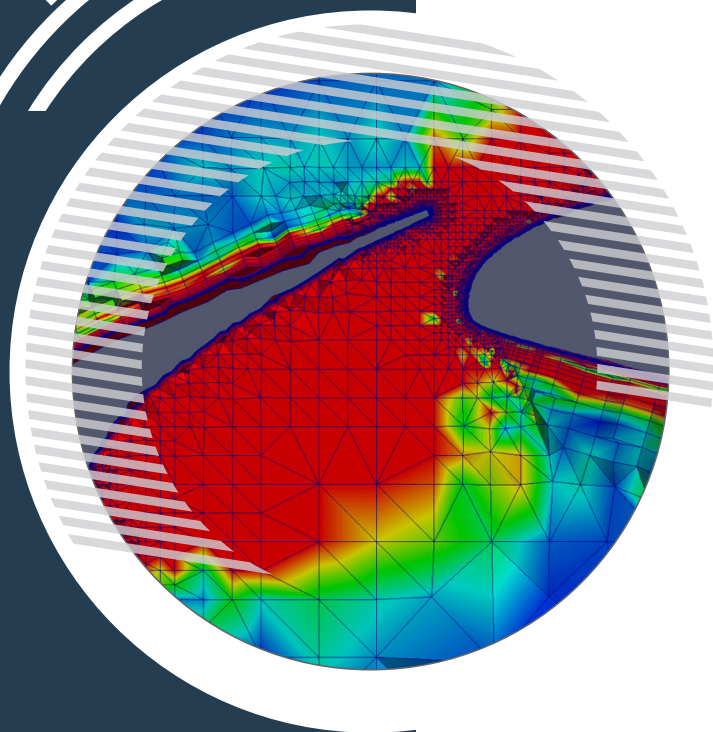
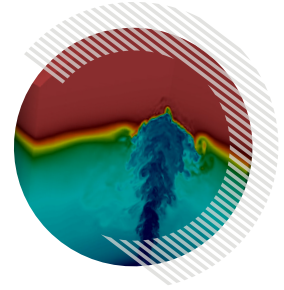


Argonne **Leadership**  
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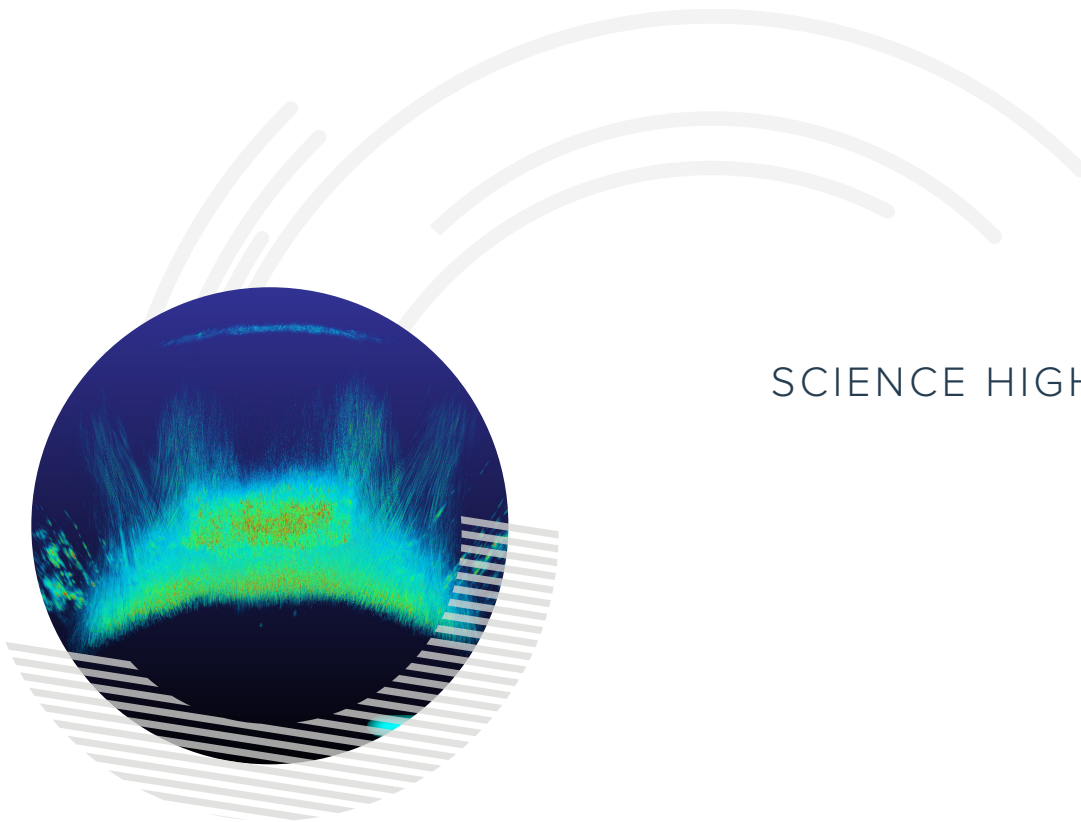


SCIENCE HIGHLIGHTS **2014**





Argonne **Leadership**  
**Computing** Facility



SCIENCE HIGHLIGHTS **2014**

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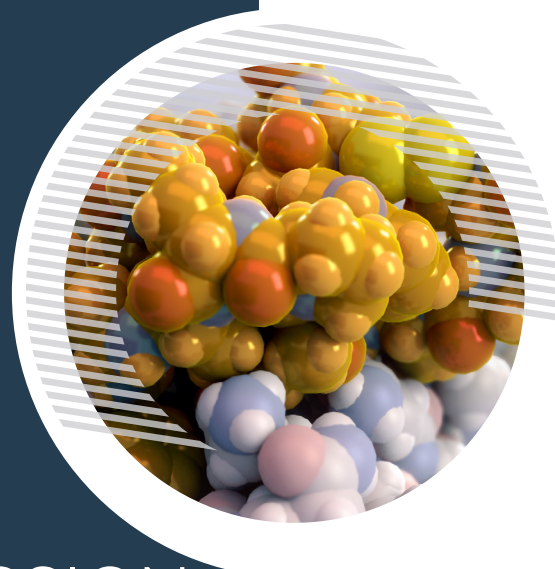
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# ABOUT ALCF

The Argonne Leadership Computing Facility provides supercomputing capabilities to researchers from national laboratories, academia, and industry to enable significant advances in science and engineering. The ALCF is supported by the U.S. Department of Energy's Office of Science, Advanced Scientific Computing Research (ASCR) program.



# MISSION

The ALCF's mission is to accelerate major scientific discoveries and engineering breakthroughs by designing and providing world-class leadership computing facilities in partnership with the computational science community.

# SCIENCE DIRECTOR'S MESSAGE

With more than a full year of Mira now in the books, we have seen significant computational science and engineering advances taking place at the ALCF. From lithium-air battery research to new insights on turbulent flows, you'll read about a sampling of our groundbreaking projects in the Science Highlights section that follows.

It has also been encouraging to see how well and how quickly our users have taken to Mira's powerful IBM Blue Gene/Q architecture. Scaling and optimization efforts have helped many important applications to achieve high levels of concurrency, which, in some cases, includes using as many 64 hardware threads per node. The ability to exploit high concurrency within a node is not only beneficial for performance on Mira, but also provides a good start for transitioning to future leadership computers, all of which will have even higher levels of concurrency per node.

While some research teams are equipped to adapt their own codes for new systems, other users have benefitted greatly from participating in our Early Science Program for Mira, attending ALCF workshops like the annual Mira Performance Boot Camp, and/or working directly with our excellent team of catalysts and performance engineers.

This year also marked the second year of the Argonne Training Program on Extreme-Scale Computing (ATPESC), an intensive two-week program I conceived to help grow the scientific computing community by training researchers to use high-end computers. Each year we've had to select around 60 participants from pools of more than 150 highly qualified applicants; the strong interest in ATPESC indicates we are filling a gap.

Many institutions offer introductory courses and some even provide advanced training programs in scientific computing, but they typically cover fewer topics in less detail. With ATPESC, our goal is to provide in-depth instruction on virtually all aspects of using leading-edge computing systems, with a strong focus on programming techniques and numerical algorithms.

We're also making an effort to extend the reach of ATPESC beyond the classroom by videotaping all of the lectures and posting them online. While viewing the lectures is no substitute for participation, we anticipate the videos will be a valuable resource to those interested in computational science and engineering.

We're already seeing how much of an impact a program like ATPESC can have. We've recently heard from some ATPESC alumni who have put their training to work. Two participants have had papers accepted in SC14's highly competitive and renowned Technical Program. Another participant is teaching a college course on high-performance computing that incorporates some of the lessons he learned at ATPESC. If our first two graduating classes are any indication, I'm pleased to say that the future of extreme-scale computing looks very bright.



**Paul Messina**  
ALCF Director of Science,  
Argonne Distinguished Fellow

# COMPUTATIONAL READINESS

## ALCF Training and Outreach Aims to Grow User Community

While the term “computational readiness” refers to a code’s ability to perform on leadership-class supercomputers, it could also be applied to the researchers carrying out the science simulations.

To make use of powerful machines like Mira with hundreds of thousands of processors, research teams must have knowledge of computer architectures, parallel programming, mathematical software, data management and analysis, performance analysis tools, software engineering, and so on.

In addition, high-performance computing (HPC) architectures evolve quickly, necessitating different code optimizations or approaches to use the new systems efficiently. Software tools and methods also change with time, requiring computational scientists to stay abreast of the latest trends and technologies in their fields.

Due to this complex and ever-changing landscape, the ALCF has taken an active role in training and outreach activities to educate computational scientists and engineers on best practices and new approaches, while also aiming to grow the HPC community by grooming the next generation of supercomputer users.



From the Argonne Training Program on Extreme-Scale Computing (ATPESC) to annual scaling workshops, the ALCF offers several expert-guided, hands-on training opportunities to inform researchers of the tools, computational resources, and services available to them in support of scientific discovery.

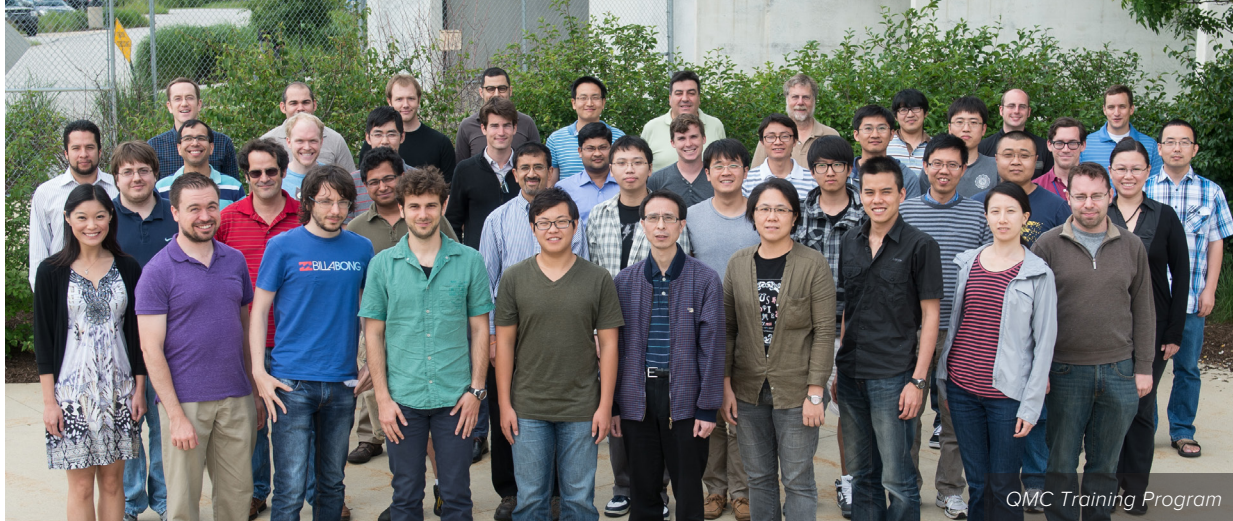
### **Building a New Generation of HPC Users, Two Weeks at a Time**

Using a supercomputer requires training far beyond what most computational science and engineering students receive. To help fill this gap, Paul Messina, director of science at the ALCF, conceived and organized ATPESC, an intense two-week program that provides in-depth training on the key skills, approaches, and tools needed to conduct research on the high-end computing systems of today and tomorrow.

Funded by the DOE’s Office of Science, this year’s event marked the second installment of ATPESC. With world-renowned HPC experts serving as the lecturers, the 62 attendees learned the ins and outs of designing, implementing, and executing large-scale computer science and engineering applications effectively and across a variety of supercomputing platforms—including methodologies expected to be applicable to future systems.

As part of the hands-on training, the participants were provided access to some of today’s most powerful supercomputing resources, including ALCF’s IBM Blue Gene/Q systems, Vesta and Mira; the Oak Ridge Leadership Computing Facility’s (OLCF) Titan system; and the National Energy Research Scientific Computing Center’s (NERSC) Edison system.





“Systems like Mira can enable breakthroughs in science, but to use them productively requires significant expertise in a number of disciplines. Our training program exposes the participants to those topics and provides hands-on exercises for experimenting with most of them,” Messina said.

For those unable to participate, videos of the 2013 ATPESC lectures are publically available at [extremecomputingtraining.anl.gov/2013-videos](http://extremecomputingtraining.anl.gov/2013-videos). Videos of the 2014 lectures will be available this fall.

### **Crash Course on Quantum Monte Carlo**

In July, the ALCF hosted a training workshop on quantum Monte Carlo (QMC), an increasingly popular computational method for chemistry, materials science, and physics research.

Designed to grow the user base of QMC, the weeklong workshop, which was supported by DOE’s Basic Energy Sciences program and the National Science Foundation, brought in 33 participants consisting of scientists, professors, and graduate students.

In the past, the QMC method was considered too difficult and computationally expensive for most researchers to use. But that has changed with the emergence of

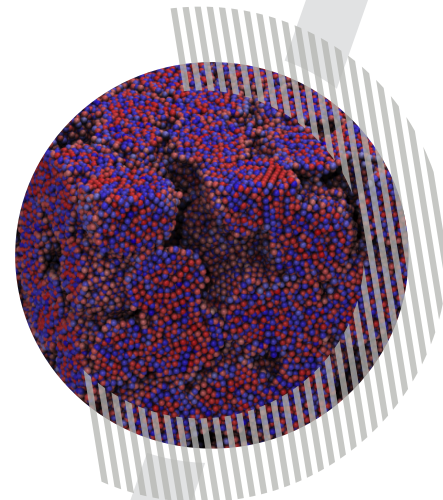
petascale supercomputers like Mira. As one of the most accurate electronic structure methods, QMC provides an important computational tool for solving many-body calculations for a broad range of electronic systems, from weakly bound molecules to strongly correlated solids.

The training program introduced participants to the fundamentals of QMC theory as well as the latest developments in QMC methods and applications. The attendees also received hands-on training using QMCPACK, an open source QMC code, on Mira.

“With this event, we set out to equip a new set of researchers to use QMC to accelerate scientific breakthroughs,” said Anouar Benali, an ALCF computational scientist who helped organize the training program.

### **Boot Camp Boosts Code Performance, Propel Science**

New and seasoned ALCF users convened at Argonne in May for the annual Mira Performance Boot Camp. For many, the primary goal of attending was to tap into the expertise of ALCF staff for assistance in improving their code’s scalability to demonstrate computational readiness for a 2015 INCITE award. In support of this goal, the ALCF’s annual scaling workshop is especially geared for and timed





to coincide with efforts of teams preparing INCITE proposals.

The bulk of the three-day event was devoted to hands-on tuning of applications. In addition, ALCF experts spoke on topics of interest, including Blue Gene/Q architecture, ensemble jobs, parallel I/O, and data analysis. Guest tool and debugger developers also provided information and individualized assistance to attendees.

With dedicated Boot Camp reservation queues, participants had quick, uninterrupted access to ALCF resources, allowing them to run nearly 400 jobs and use over 1.7 million core-hours as they diagnosed code issues and tweaked performance.

Even tried-and-true codes benefitted from the intense support at Boot Camp, including NCAR's Community Earth System Model, which is being used for the INCITE project, CESM Century-Scale Climate Experiments with a High-Resolution Atmosphere (PI: Warren Washington).

“Our model has already been tuned extensively, so the improvements we made were totally unexpected. The 30 percent speedup means we can get 30 percent more science from our INCITE allocation,” said Adrienne Middleton, software engineer at NCAR.

### **Virtual Training Extends ALCF's Reach**

In 2013, the ALCF transitioned its Getting Started program from an on-site event to an interactive virtual webinar. With the convenient online format, new users from around the globe are able to log in remotely to learn about ALCF services and resources, get details of the IBM Blue Gene/Q architecture, and receive guided assistance in porting and tuning applications on Mira.

Getting Started class sizes are kept small to emulate an intimate classroom experience that includes hands-on exercises. Session offerings are timed to coincide with INCITE and ALCC award announcements when many projects add new users. This just-in-time training maximizes research on ALCF resources by facilitating and encouraging early utilization of allocations. To further accommodate new user needs, a video presentation of this popular training course is also available for viewing on the ALCF website.

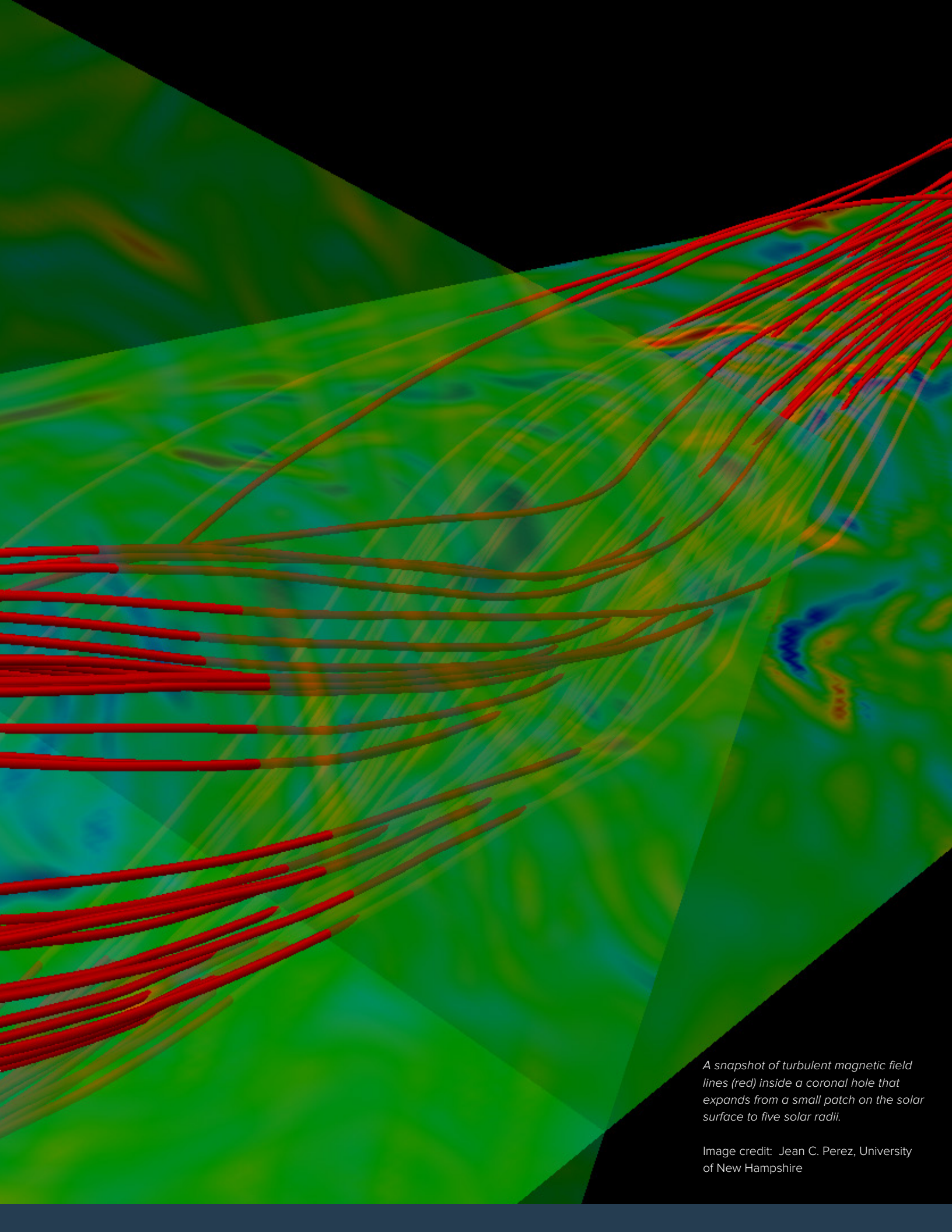
### **Collaborating with Peers to Improve User Experience**

The ALCF also collaborates with peer DOE institutions to develop training opportunities, explore key technologies, and share best practices that improve the user experience.

In June, for example, leaders from many national computing facilities convened in Oakland, CA for the Joint Facilities User Forum on Data-Intensive Computing. Organized by Argonne, Oak Ridge, Lawrence Berkeley, Sandia, Lawrence Livermore, and Los Alamos national laboratories, the three-day workshop brought together facility users and HPC center staff to discuss the latest trends and techniques related to data management, analysis, and visualization. Building on the momentum of this successful conference, ALCF and its co-organizers are planning more user-focused events, including virtual workshops for DOE facility users and staff.

In addition, ALCF, OLCF, and NERSC staff are working together to develop strategies to ensure key applications are ready for the scale and architecture of the next generation of DOE supercomputers. Using the ALCF's Early Science Program for Mira as a model, this effort aims to ensure scientific applications are ready to run on diverse next-generation supercomputer architectures.





*A snapshot of turbulent magnetic field lines (red) inside a coronal hole that expands from a small patch on the solar surface to five solar radii.*

Image credit: Jean C. Perez, University of New Hampshire

# ALLOCATION PROGRAMS

**Any researcher in the world with a large-scale computing problem can apply for time on ALCF computing resources. Project proposals are peer-reviewed and assessed for computational readiness. Accepted projects are allocated parcels of computing time that add up to billions of core-hours each year.**

## INNOVATIVE & NOVEL COMPUTATIONAL IMPACT ON THEORY AND EXPERIMENT (INCITE)

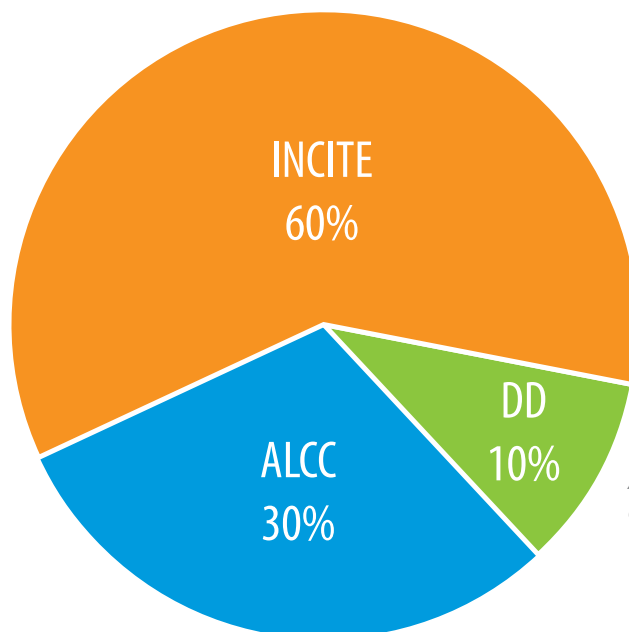
The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering. The program conducts a two-part review of all proposals: a peer review by an international panel of experts and a computational-readiness review. The annual call for proposals is issued in April and the allocations are awarded in millions of core-hours for one to three years.

## ASCR LEADERSHIP COMPUTING CHALLENGE (ALCC)

The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources. The DOE conducts a peer review of all proposals based on scientific and technical merit of the project; appropriateness of the proposed method or approach; competency and adequacy of personnel and proposed resources; and the reasonableness and appropriateness of the proposed allocation request. The yearlong allocation cycle runs from July 1 to June 30.

## DIRECTOR'S DISCRETIONARY (DD)

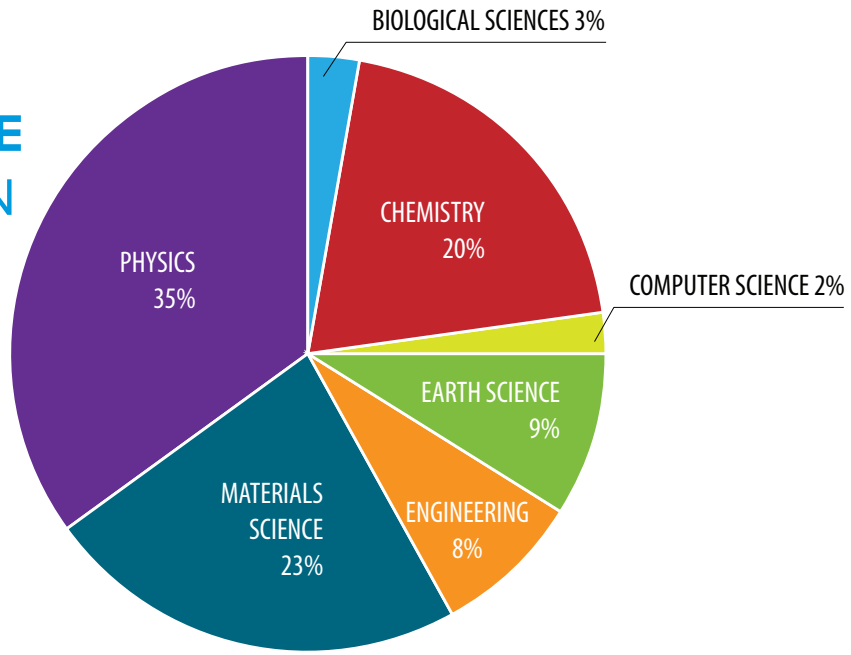
The ALCF's DD program provides "start up" awards to researchers working toward an INCITE or ALCC allocation to help them achieve computational readiness. Projects must demonstrate a need for leadership-class resources. Awards may be made year round to industry, academia, laboratories, and others, and are usually between three and six months in duration. The size of the award varies based on the application and its readiness/ability to scale; awards are generally from the low hundreds of thousands to the low millions of core-hours.



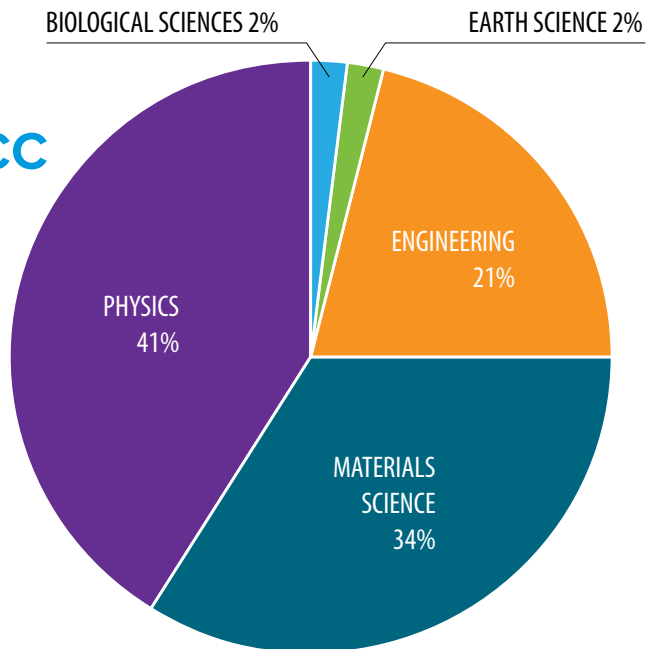
*A breakdown of how ALCF computing time is allotted among the three allocation programs.*



## 2014 INCITE BY DOMAIN



## 2013-2014 ALCC BY DOMAIN



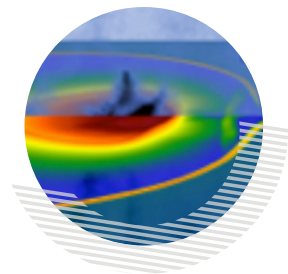
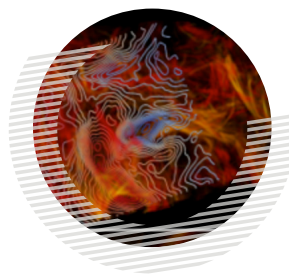
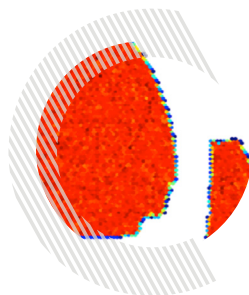
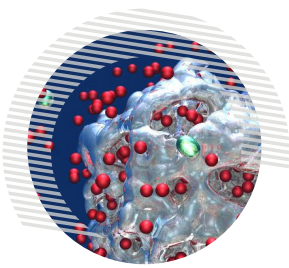
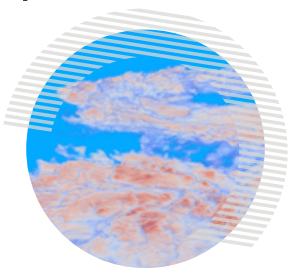
# CONTINUING DISCOVERIES

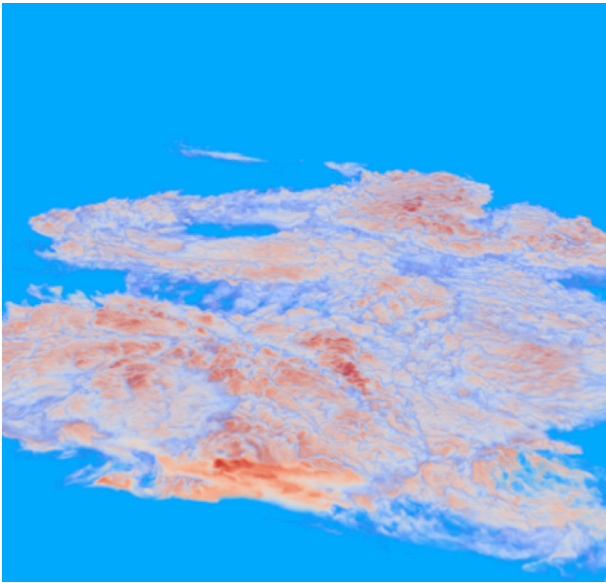
## PAST PROJECTS PROVIDE VALUABLE INSIGHTS

Supercomputers are powerful research tools that can greatly accelerate scientific discoveries, but analyzing the massive datasets they produce is a process that can take many months. In fact, several projects at the ALCF are so innovative and complex that it can take years to fully develop the necessary software and achieve research goals.

In addition, ALCF users often seek allocation renewals to continue their work from year to year, allowing research projects to evolve along with the facility and its increasingly powerful computing resources. In the following pages, we highlight some past projects that have achieved notable results.

14





*Rendering of ice mixing ratio in one hour-old contrail cirrus in a 10 km x 10 km x 4 km computation domain. Levels are in the range 1 mg/kg (blue) to 25 mg/kg (red). Atmospheric turbulence and radiative transfer modules are activated (day conditions). The simulations were carried out with the code Méson-NH on Intrepid, the ALCF's now-decommissioned IBM Blue Gene/P supercomputer.*

Image credit: Roberto Paoli and Odile Thouron, CERFACS

## Evaluation of Mesoscale Atmospheric Model for Contrail Cirrus Simulations

Contrails, the visible white lines in the sky left behind airplanes, are ice clouds made of water exhaust from the aircraft's engine. Contrails can spread to form cirrus clouds that affect the Earth's radiation budget. As the volume of air travel continues to grow, the impact of contrail cirrus is of increasing concern to scientists and policymakers.

A research team from the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) is using ALCF computing resources to fine-tune numerical models that will allow for a more accurate understanding of the impact of contrail cirrus on global climate. With an earlier INCITE award, the researchers used high-resolution large eddy simulations to characterize the mechanisms that control the transition from the contrail stage to the young cirrus stage as a function of the wake age. They observed that atmospheric turbulence is the main driver of contrail evolution after vortex breakup, whereas at later stages, radiative transfer and sedimentation affect the transition by controlling the horizontal and vertical spread of the plume.

With their 2013 INCITE allocation, the researchers examined contrail evolution up to one hour after emission. One important result of the study is that radiative transfer is the key mechanism controlling the global ice characteristics and the vertical extension of the contrail, while atmospheric turbulence no longer has a significant impact on contrail evolution one hour after the contrail has formed. The effect of radiative transfer is magnified during the day due to direct heating at the top of the contrail, which also adds to the heating caused by the Earth's surface at the bottom of the contrail. The team is now using a Director's Discretionary allocation at the ALCF to carry out a detailed analysis of microphysical and optical properties of contrails, and to propose parameterizations of these quantities for global and climate models.

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2013 INCITE | 240 Million Core-Hours

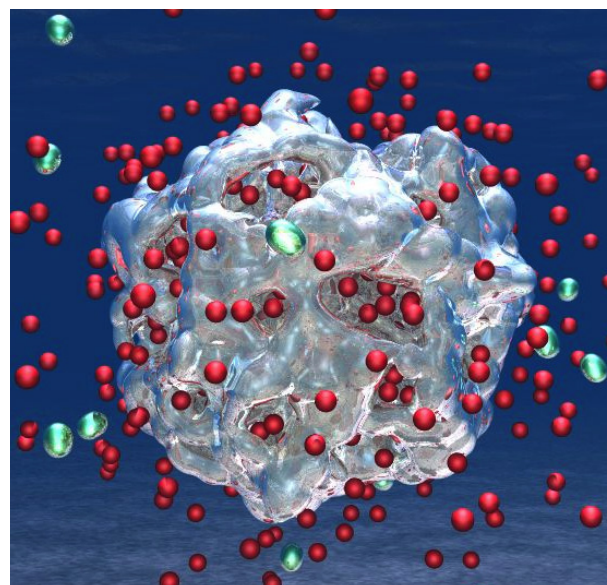
## Petascale Simulations of Stress-Corrosion Cracking

In the final year of this three-year INCITE allocation, University of Southern California (USC) researchers performed quantum molecular dynamics (QMD) simulations to study the reaction of a lithium-aluminum (Li-Al) alloy particle with water for rapid, high-yield hydrogen production. The team previously used the allocation to investigate fundamental mechanisms of stress-corrosion cracking, nanoindentation of amorphous silica in the presence of water, and impurity segregation-induced embrittlement of metallic alloys.

Producing hydrogen from aluminum-water reactions has potential for clean energy applications, including on-board fuel production for hydrogen-powered vehicles, but the process has been limited by its low reaction rate and poor yields. However, recent experiments have suggested that alloying aluminum with lithium could help overcome these issues. With their INCITE award, the USC research team used Mira to shed light on the atomistic mechanisms of this promising approach.

The researchers performed a 16,611-atom QMD simulation that revealed alloying aluminum particles with lithium results in orders-of-magnitude acceleration of the reaction rate, as well as higher yield. Their simulations also helped identify the key mechanisms underlying this rapid, high-yield reaction. The mechanisms included having efficient charge pathways in the aluminum atoms that collectively act as a “superanion,” and the dissolution of lithium atoms into water to produce a corrosive basic solution that prevents the formation of a reaction-stopping passive oxide layer on the particle surface.

Scalability is another major obstacle to using aluminum particles for hydrogen production. Namely, the high reactivity of aluminum particles cannot be sustained for larger particles that are commercially mass produced. To investigate the scalability of the process, the researchers compared simulations involving  $\text{Li}_{135}\text{Al}_{135}$  and  $\text{Li}_{441}\text{Al}_{441}$  in water (total of 4,836 and 16,611 atoms, respectively). They found these surfaces were equally reactive regardless of the surface curvature, indicating the alloy design has the potential to scale up to industrially relevant particle sizes.



*Hydrogen production from water using a  $\text{Li}_{441}\text{Al}_{441}$  particle. The valance electron density represented by the silver isosurface is centered around Al atoms, whereas some of the Li atoms represented by red spheres are dissolved into water. Produced hydrogen molecules are represented by green surfaces. Water molecules are not shown for the clarity of presentation.*

Image credit: Rajiv Kalia, Aichiro Nakano, Ken-ichi Nomura, and Priya Vashishta, University of Southern California; Kohei Shimamura and Fuyuki Shimojo, Kumamoto University, Japan

Acknowledgment: Dr. James Davenport, Program Manager of Theoretical Condensed Matter Physics, Division of Materials Science and Engineering, BES (Grant Number DE-FG02-04ER46130) supported this research. Computing resources for this DOE-supported research were provided by the INCITE program.

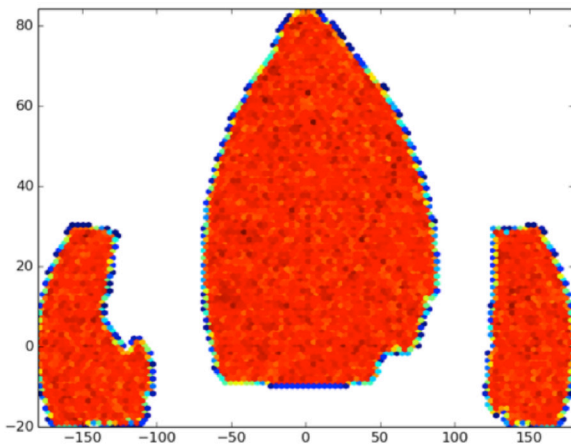
## Physics

**SALMAN HABIB**

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2013 INCITE | 40 Million Core-Hours



*The areal density of emission line galaxies from mock catalogs produced for the DESI experiment. These mock catalogs are being used to test fiber assignment algorithms and optimize the DESI footprint and survey strategy.*

Image credit: Martin White,  
University of California, Berkeley

## Computing the Dark Universe

With research that began on Mira with the ALCF's Early Science Program in 2012, this project has been critical to planning for the Dark Energy Spectroscopic Instrument (DESI), a DOE cosmological survey that will measure the impact of dark energy on the expansion of the universe, starting in 2018. A team of researchers from Argonne and the University of California (UC), Berkeley, continues to use results from the world's largest high-resolution cosmological simulation, known as the Outer Rim simulation, to help optimize and design the DESI survey strategy and footprint.

The massive Outer Rim simulation provides a unique resource worldwide that matches the remarkable depth and volume of the DESI survey. Covering a large portion of the observed universe, the simulation resolves the dark matter halos that host the galaxies and quasars to be observed by DESI, including luminous red galaxies and emission line galaxies. Carried out on Mira with HACC (Hardware/Hybrid Accelerated Cosmology Code), the simulation was run on 32 racks, or two-thirds of the full machine.

To achieve the required resolution, the Outer Rim simulation modeled the evolution of more than one trillion particles in a volume of 4,225 Mpc on a side. From the simulation, 100 full snapshots are stored, each encompassing 40 TB of raw data (particle positions, velocities, and tags). With these snapshots, which comprise a movie of the universe, the researchers are able to extract details of the evolution of its structure and use the information to decide what galaxies are hosted by different mass halos.

For one major task, the team worked to add galaxies to the resulting simulations. First, they identified the dark matter clumps that form in the simulation using a halo finder. Like the main simulation, this step also required using 32 racks of Mira. Guided by already available observational data, researchers from UC Berkeley then populated the halos with the different galaxies relevant for the DESI survey. Finally, the resulting galaxy and quasar catalogs were employed by the DESI observational team at Lawrence Berkeley National Laboratory to optimize the survey footprint and observational strategy, as well as the optical fiber assignment algorithms for the observations.

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2013 INCITE | 53 Million Core-Hours

## Petascale Simulations of Inhomogeneous Alfvén Turbulence in the Solar Wind

This multi-year INCITE project aims to advance understanding of Alfvén wave turbulence in the inner heliosphere and the role that it plays in the heating and acceleration of the solar wind. Turbulence in any context is challenging to describe due to its complex, nonlinear nature. In the solar wind acceleration region, there is the additional challenge that background solar wind properties, including density, solar wind outflow velocity, and magnetic field strength, are highly inhomogeneous. These inhomogeneities lead to wave reflections that trigger a turbulent cascade, called reflection-driven turbulence.

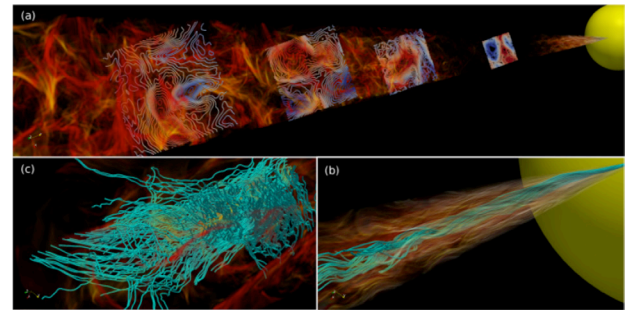
To advance our understanding of Alfvén turbulence in an inhomogeneous background, the INCITE research team is conducting large numerical simulations with their inhomogeneous magnetohydrodynamics (MHD) code, called REFLECT. Combined with the petascale power of Mira, the code allowed researchers to resolve both the inhomogeneity of background profiles and the small-scale structures that result from the turbulent dynamics.

One of the project's most important recent accomplishments was the successful completion of an unprecedented simulation using a fine mesh of 8.6 billion points, which approximated a magnetic flux tube extending one-third the distance of the Sun to the Earth. The results from this simulation provide new evidence of the formation of a  $1/k$  energy spectrum similar to that observed in the solar wind by *in situ* measurements of earlier Helios space probe missions.

While there has been significant debate as to the spectrum's origins, the simulations show evidence that reflection-driven turbulence can indeed lead to a flat spectrum by a local mechanism and can be directly compared to existing observations of the Helios mission. These findings are the first observations of a  $1/k$  spectrum of Alfvén waves in direct numerical simulations of MHD turbulence, which provides the simplest framework to describe magnetized plasma turbulence.

Not only is this project making significant contributions to the fundamental aspects of MHD turbulence, the results will also lead to transformative advances in determining the viability of Alfvén wave turbulence as a major mechanism for the heating of the solar corona and the acceleration of the solar wind. In addition, Alfvén waves and

Alfvén turbulence are ubiquitous in a number of other magnetized plasmas and play a significant role in a variety of other astrophysical and laboratory processes.



(a) Large-scale Alfvén waves, shown as contour lines at selected radii, transport energy from the solar surface into the solar atmosphere along a coronal hole. The waves become turbulent and heat the ambient plasma in small-scale turbulent structures, shown in the orange gray scale. (b) Magnetic field line rendering near the sun. (c) Turbulent magnetic field lines above 60 solar radii, covering the lowest orbit of the Helios mission.

Image credit: Jean C. Perez, University of New Hampshire



## Physics

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2013 INCITE | 40 Million Core-Hours

## Transformative Simulation of Shock-Generated Magnetic Fields

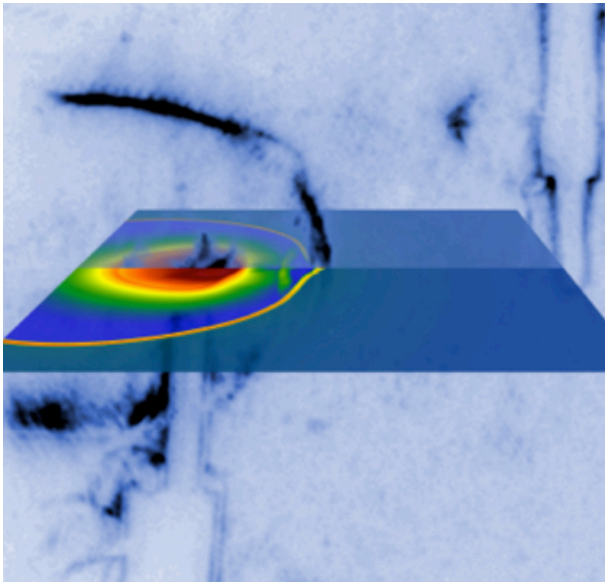
Magnetic fields are present throughout the universe and can play many and varied roles in astrophysical processes. The origins of these fields and the required mechanisms for their amplification have been a long-standing subject of interest in astrophysics. With this INCITE project, researchers from the Flash Center for Computational Science at the University of Chicago have developed high-fidelity numerical models that provide crucial insights into the physical processes involved in magnetic-field generation.

Their work at the ALCF contributes to the efforts of an international team of theoretical and experimental physicists studying Cassiopeia A, a supernova remnant some 11,000 light years from Earth, which was first observed over 300 years ago. The shock wave generated by its explosion continues to expand and serves as the source of bright radio emissions believed to be instigated by an intense magnetic field within the cluster of gaseous star debris.

Researchers across the world are working to confirm that these inner magnetic fields are amplified by turbulence within the remnant, making them 100 times more powerful than those just beyond the shock rim. This turbulence may occur when ejecta from the shock wave passes through and interacts with dense clumps of stellar matter surrounding Cassiopeia A.

Recently, a team led by researchers at Oxford University came a step closer toward proving this theory in a laboratory experiment that recreated a supernova explosion by concentrating three high-intensity laser beams on a carbon rod and detonating it in a chamber of low-density argon gas. *In situ* measurements confirmed that the magnetic field was amplified in the turbulent wake caused by the laser-produced shock.

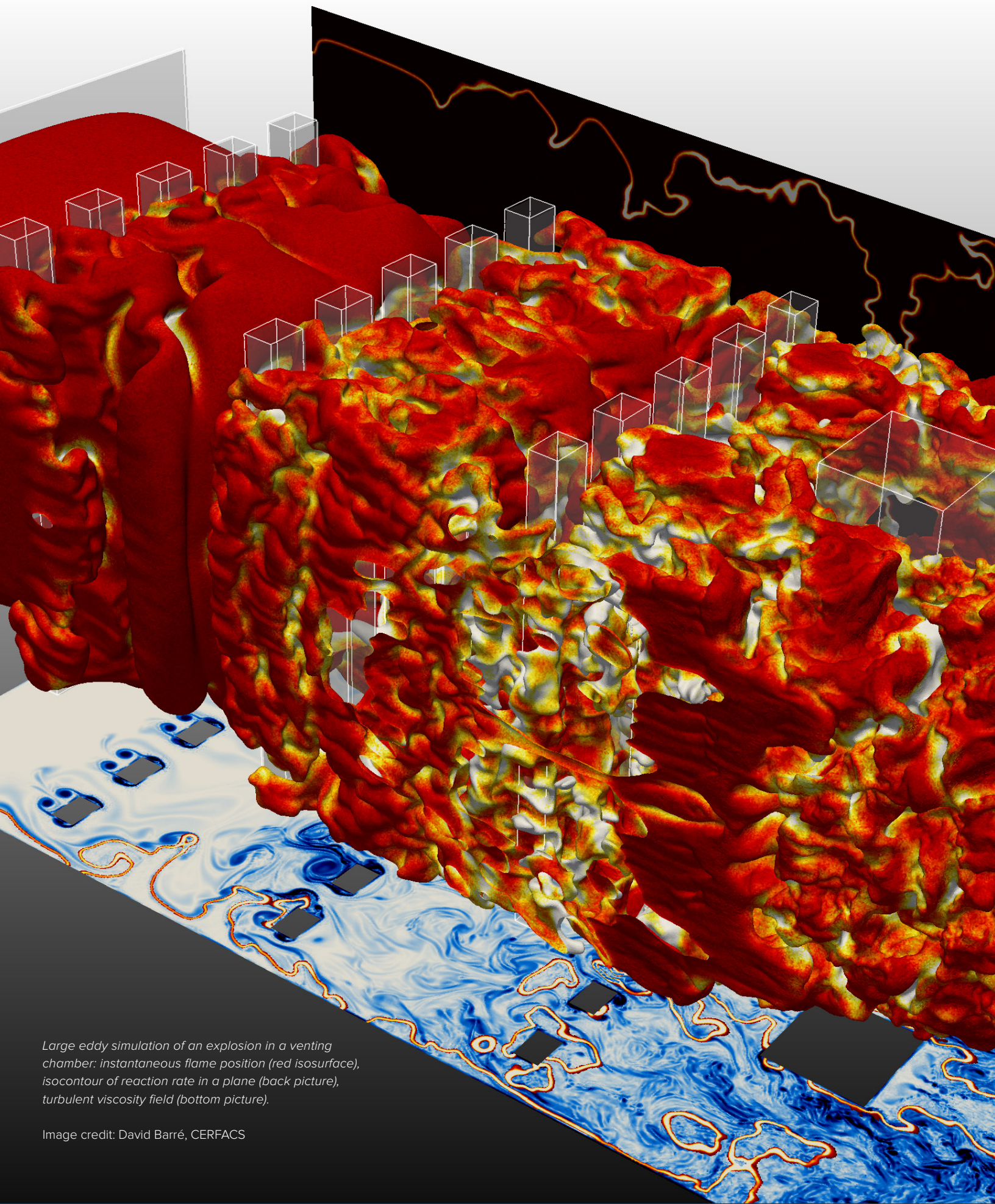
At the ALCF, the University of Chicago research team used the FLASH code, an open source finite volume code with an extended range of physics capabilities, to perform high-fidelity simulations designed to interrogate the laboratory experiment. This allowed them to disentangle the physics in play and explain the experimental results, while also matching the diagnostic measurements. The numerical models developed during this project are also expected to assist future experiment designs and, ultimately, help tackle the two-fold problem of magnetic field generation and turbulent amplification.



*Composite image combining experimental data (Schlieren imaging) and numerical results (density logarithm). A carbon rod target is illuminated with a 300J laser for 1ns, which forms an asymmetric shock-front in the argon gas. The self-generated magnetic field is measured at late times using a "Bdot" probe, seen on the right.*

Image credit: Petros Tzeferacos, University of Chicago; Gianluca Gregori and Jena Meinecke, Oxford University



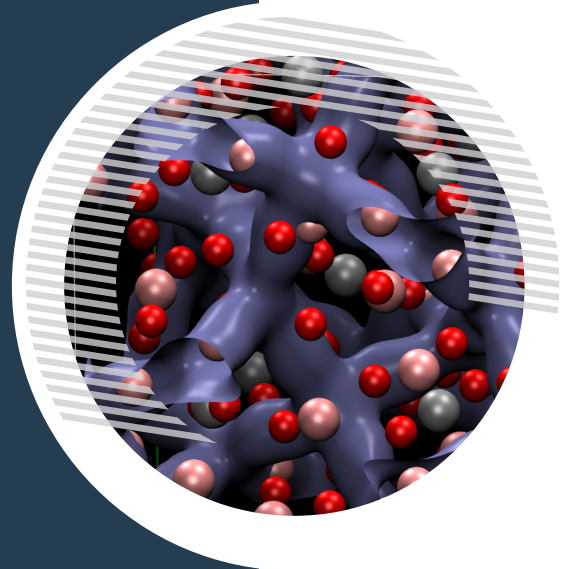


*Large eddy simulation of an explosion in a venting chamber: instantaneous flame position (red isosurface), isocontour of reaction rate in a plane (back picture), turbulent viscosity field (bottom picture).*

Image credit: David Barré, CERFACS



# SCIENCE HIGHLIGHTS



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 National Cancer Institute  
 Director's Discretionary | 4 Million Core-Hours

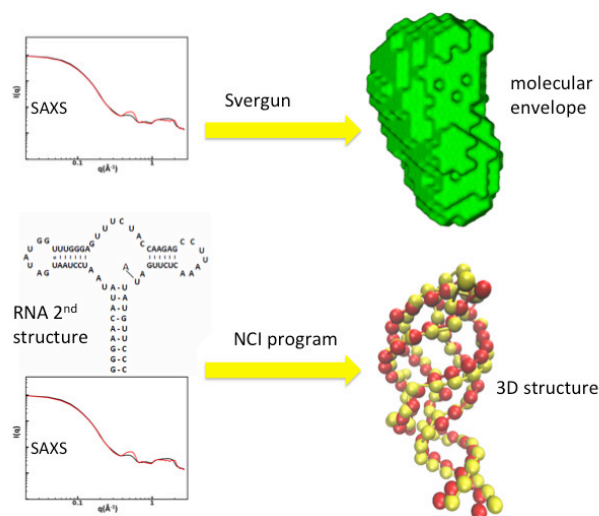
## Computing 3D Structures of Large RNA from Small-Angle X-ray Scattering Data and Secondary Structures

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

The Protein Data Bank is a worldwide repository of information on the 3D structures of large biological molecules. Currently, proteins make up a vast majority of the repository, with RNA structures accounting for less than three percent of the entries. This disparity can primarily be attributed to technical challenges in determining RNA structures with existing methodologies. New approaches and tools are required for structure determination of large RNA.

With a Director's Discretionary allocation at the ALCF, the NCI research team is developing a robust algorithm and computational program to calculate 3D structures of RNA using small-angle X-ray scattering (SAXS) data and known secondary structures as input. To conduct these types of calculations, the researchers need to generate tens of thousands of structures for each type of RNA. The goal of the project involves computing the structures of RNAs with various folds and complexities, which necessitates the use of a petascale supercomputer like Mira.

In collaboration with ALCF researchers, the team is working to scale and optimize the code to prepare for a more substantial allocation on Mira in the future. This effort includes parallelizing the code with MPI, which will allow them to perform tens of thousands of concurrent Monte Carlo trial moves in a 3D configuration space of RNA. ALCF staff further helped improve the OpenMP implementation by optimizing the dynamic schedule of OMP chunks. The current hybrid MPI/OMP code can linearly scale to 64 threads per node, which is ideal OMP scaling for Mira's IBM Blue Gene/Q architecture.



*This figure compares the Svergun method, which generates a molecular envelope, with the NCI research team's newly developed method to determine 3D structure. The RNA molecule in this illustration is a 71-residue RNA. The red and yellow spheres represent residues in crystal and calculated structures.*

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

### IMPACT

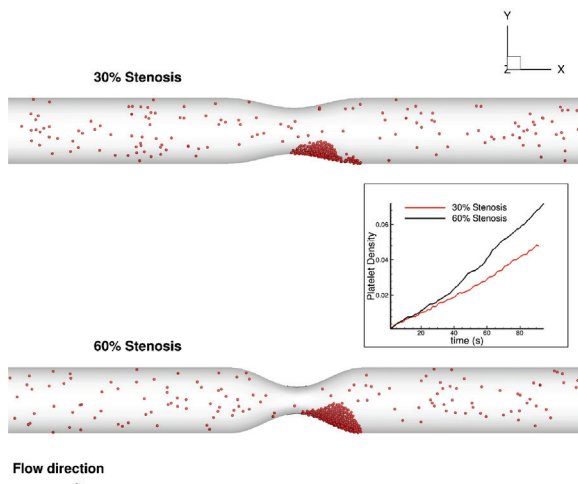
**This project aims to develop a combined computational and experimental approach to determine RNA in-solution structures, which is key to understanding the many biological functions of RNA. The hope is that this tool will provide researchers with information that will help improve the diagnosis and treatment of cancer and other diseases.**

**GEORGE KARNIADAKIS**

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INCITE | 45 Million Core-Hours



*Platelet aggregation in a stenosis: snapshots of the thrombus at time  $t = 90$  sec for two geometries at different stenosis levels of 30 percent and 60 percent. Aggregation is initiated by seeding activated platelets downstream of the stenosis apex. Inset shows the time evolution of thrombus formation.*

Image credit: George Karniadakis, Brown University

## Multiscale Simulations of Human Pathologies

Thoracic aortic aneurysm and dissection (TAAD) occurs when an aneurysm in the aorta expands and causes a tear in the artery wall. To help better understand and treat this life-threatening condition, researchers from Brown University are using Mira to perform pioneering multiscale simulations of the biophysical features of TAAD.

TAAD is estimated to be responsible for around 30,000 deaths per year in the U.S. alone, but the condition is still not well understood. However, recent advances in genetics and medical imaging have resulted in a significant increase in the number of diagnosed TAADs and an increased appreciation of the roles played by thrombi (blood clots) in aortic dissections.

Building on extensive computational expertise and past INCITE awards, the Brown University research group has developed a flexible approach that integrates multiple computer codes to perform truly multiscale simulations of realistic biological systems. They are currently using this approach on Mira to conduct the first simulations of the hemodynamic conditions under which thrombi form in aortic dissections, and the biomechanical consequences of thrombi on the artery wall.

The research team has developed and validated a model for platelet aggregation in blood using the dissipative particle dynamics method. They are using this model to investigate the effect of different geometries on platelet aggregation by considering arterial stenosis at different levels of occlusion, and aneurysms of different shapes and sizes.

Thus far, the team has studied platelet aggregation growth rates by simulating blood flow in a microvessel at different flow rates. The simulations predicted thrombus growth with shapes and patterns similar to those observed experimentally. Their work has also indicated that activation delay time plays a significant role in determining the thrombus size and the shear rate at which the maximum growth rate occurs. Additionally, the researchers have established a pipeline from mouse-specific experimental data to continuum modeling of flow-structure interactions by performing simulations of mouse aortas.

### IMPACT

**By significantly increasing our understanding of TAADs, this research could lead to an improved prognostic capability and interventional planning. In addition, insight gained in this study will have important implications for a host of other vascular conditions, providing information that could contribute to improved treatments for a broad class of clinical problems.**

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ALCC | 22.8 Million Core-Hours

## Protein Binding and Interaction Analysis of Human Pathogen Protein Targets

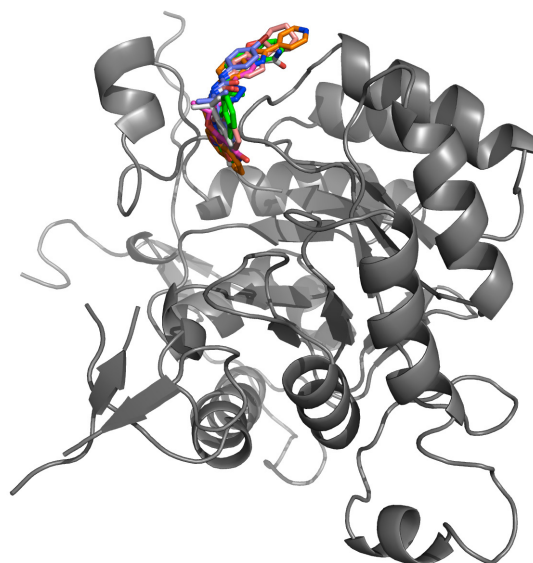
As pathogens evolve and become more resistant to known antibiotics, global healthcare threats are imminent. Better understanding of the interactions between proteins and small drug-like molecules is important in the development of strategies to react to antibiotic resistance. This study will apply state-of-the-art methodologies toward studying ligand-protein interactions, specifically on important protein targets from human pathogens that represent potential drug targets.

Historically, computer-based drug discovery efforts benefit significantly from the presence of a ligand-protein complex. Computational discovery studies conducted throughout this project will help researchers understand the role of ligand-protein interactions in human pathogens, bioterrorism agents, and human disease-related proteins.

At its computational core is the Analysis Pipeline for Protein Ligand Interaction and Enzymatic Design (APPLIED), a hierarchical, multistate pipeline combining molecular modeling, docking, and free binding energy calculations. Operating on Mira, APPLIED provided valuable biological insights on important protein targets in infectious diseases. This included the identification of nine novel inhibitors against the enzyme inosine-5'-monophosphate dehydrogenase (IMPDH), which represents a potential pathway to treat the deadly anthrax infection.

Researchers also have focused on identifying inhibitors against New Delhi Metallo- $\beta$ -lactamase (NDM-1). The recent discovery and dissemination of the plasmid NDM-1 gene harbored by multiple pathogenic microorganisms presents a global healthcare threat. While the carbapenem class of  $\beta$ -lactam antibiotics is one of the last lines of defense against multiple and extensive drug resistant infections, their integrity has been compromised by a number of  $\beta$ -lactamases with the ability to inactivate all classes of  $\beta$ -lactam antibiotics.

The development of novel inhibitors against the antibiotic resistant protein NDM-1 has been ongoing for almost two years. In this time, research has determined the crystallographic model of the enzyme and has exhaustively studied the modes of interaction. Concurrently, collaborators have been conducting high-throughput screening experiments to identify compounds with inhibitory activity.



*Novel inhibitors targeting the IMPDH protein from human pathogen B. anthracis were discovered through a combination of state-of-the-art molecular modeling and experimental crystallography performed at the Midwest Center for Structural Genomics at Argonne National Laboratory.*

Image credit: T. Andrew Binkowski, Argonne National Laboratory

### IMPACT

**The results of this research will provide a better understanding of the mechanism and evolution of antibiotic resistance in the NDM-1 gene, and produce the critical initial data necessary to drive aggressive structure-based drug discovery efforts for NDM-1 and IMPDH.**

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INCITE | 55 Million Core-Hours

## Studies of Large Conformational Changes in Biomolecular Machines

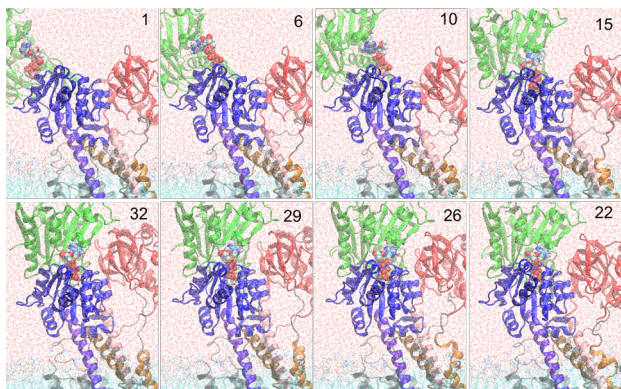
Complicated macromolecular machines abound in biology. The concerted action of these “molecular machines” underlies all the activities of the living cell. This research aims to gain a mechanistic understanding of the character of the free energy landscape that governs the function of large biomolecular systems, and demonstrate the feasibility of an extremely scalable computational strategy built upon the string method and classical molecular dynamics.

A machine is generally perceived as an intricate device comprised of different moving parts, able to utilize energy to perform some useful work. In biology, these machines are complex macromolecular assemblies of proteins, nucleic acids, and carbohydrates that consume energy in order to perform specific biological functions.

Biophysicists from the University of Chicago are continuing previous INCITE efforts to elucidate the mechanisms of complex membrane proteins through a modified version of the nanoscale molecular dynamics (NAMD) code, ported to Mira.

The resulting simulations provide a deep mechanistic perspective of protein function, linking structure to dynamics by characterizing the free energy landscape, or potential of mean force, that governs key functional motions. In the case of the protein c-Src tyrosine kinase, the effects of its regulatory domains on the activation transition were studied using the string method with swarms-of-trajectories, which requires a set of collective variables to define the transition path.

Understanding the detailed molecular mechanism of ion pumps has been a long-standing problem. Project researchers recently studied large domain motions in adenosine triphosphate (ATP)-driven ion pumps, where the first leg of the catalytic cycle has been characterized. They found that the cycle, or transition, is responsible for occlusion of calcium ions in the transmembrane binding sites, which is a crucial step in the active transport of ions against the concentration gradient.



*Movements of cytoplasmic domains of SERCA along the transition pathway from the E1-2Ca to E1-2Ca-ATP states calculated by string method with swarms-of-trajectories. The pathway is composed of 32 images of the system. Indices on the individual panels give the image indices of a few selected images along the pathway.*

Image credit: Avishek Das,  
University of Chicago

### IMPACT

**Results from this project will help develop a roadmap for simulating, visualizing, and elucidating the workings of complex molecular machines using extremely scalable computational strategies on leadership-class resources.**

**It will also assist in the rational design of novel drugs for neurodegenerative diseases, such as Parkinson's.**



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INCITE | 250 Million Core-Hours

ALCF 100 Million; OLCF 150 Million

## Computational Actinide Chemistry: Reliable Predictions and New Concepts

Computational chemistry and materials science techniques are being used to predict the properties of compounds containing heavy elements, which play a role in nuclear fuel development, cleanup, and safety. Understanding the chemistry of the actinides is among the core issues that must be addressed in order to develop appropriate technologies.

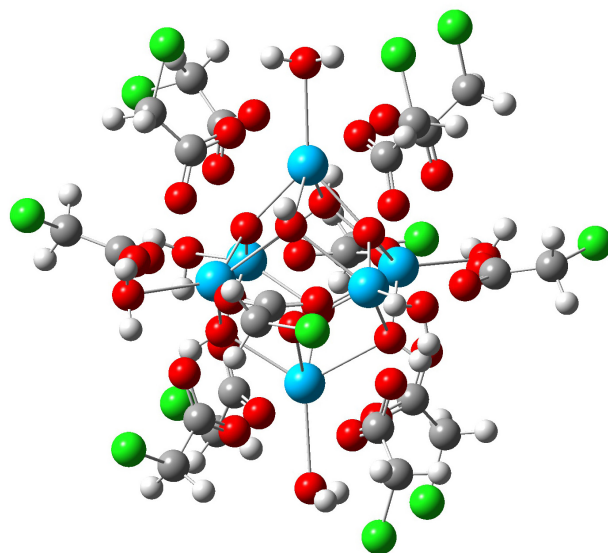
The accurate calculation of the electronic structure, energetics, and spectroscopic properties of heavy element compounds is difficult and computationally demanding. Yet, the difficulty and expense in doing experiments on radioactive materials makes simulation a critical component of any program in actinide science to improve safety and reduce costs.

The goal of this project is to obtain the first highly accurate, extrapolated, complete basis set results for actinide compounds that will serve to explain important experimental results. Large-scale, coupled-cluster single, double, and approximate triple excitation (CCSD(T)) calculations and molecular dynamics simulations have been used to study actinide complexes in various oxidation states in solution, at interfaces, and at the nanoscale. This will lead to unprecedented new insights into the behavior of these important molecular systems in complex environments.

More approximate methods, such as density functional theory, will be carefully benchmarked and used to study much larger systems, including explicit solvation effects. Further study of how actinide nanoparticles are formed in hydrolysis reactions has implications in the development of new fuel particles.

Efforts to find replacement materials for rare-earth magnets have initially focused on determining appropriate software to compute the magnetic anisotropy energy (MAE), as a surrogate for the coercive energy of the magnet. This, together with its total moment, determines the suitability of the material as a potential replacement. Initial studies of yttrium, lanthanum, and thorium cobalt compounds have shown reasonable agreement with experimental MAE trends.

This benchmark study has provided significant insight into the computational requirements for an accurate prediction of their magnetic properties.



*Density functional theory-optimized structure for  $\text{Th}_6(\text{OH})_4\text{O}_4(\text{H}_2\text{O})_6(\text{ClCH}_2\text{COO})_{12}$ . INCITE resources are being used to study how this structure forms starting from  $\text{Th}(\text{H}_2\text{O})_9^{4+}$  with  $\text{ClCH}_2\text{COO}^-$  counterions in aqueous solution.*

Image credit: Karah Knope and Lynne Soderholm, Argonne National Laboratory; David Dixon and Monica Vasiliu, University of Alabama

**IMPACT**

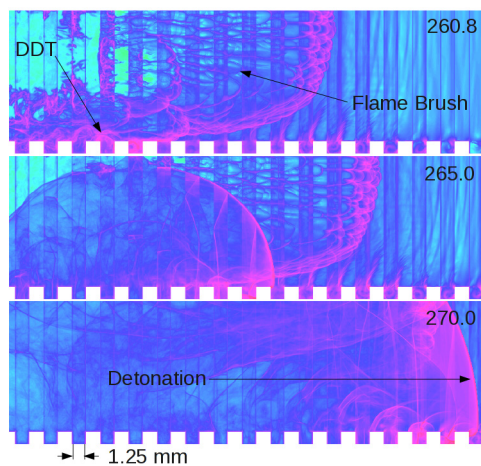
**Modeling and simulation will be critical to the cost-effective development of next-generation nuclear reactor technologies, DOE cleanup efforts, and the replacement of rare-earth magnets, which play an important role in many energy technologies.**

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INCITE | 150 Million Core-Hours



*A DNS simulation of the onset of a detonation in  $2\text{H}_2+\text{O}_2$  at initially 1 atm. pressure in a 2.5 cm square pipe with 1.25 mm grooves. The figure shows a computer-generated pseudo-Schlieren image of the density field. The gas has been ignited at the closed end of the tube (to the left of the image) and propagates to the right. The DDT takes place inside the flame brush close to one of the side walls.*

Image credit: Charles Bacon and Marta Garcia, Argonne National Laboratory; Alexei Khokhlov, University of Chicago; Joanna Austin and Andrew Knisely, University of Illinois at Urbana-Champaign

### IMPACT

**By better understanding the complex mechanisms involved in the detonation of reactive gases, researchers and engineers will be able to better predict the onset of detonation and develop safety mechanisms for real-world applications.**

## First-Principles Simulations of High-Speed Combustion and Detonation

Detonation waves caused by deflagration-to-detonation transition (DDT) in gaseous mixtures may have catastrophic consequences in a variety of industrial and energy-producing settings. This project is a systematic first-principles study of combustion and detonation phenomena in hydrogen-oxygen mixtures and other reactive gases, utilizing direct numerical simulations (DNS) to gain a fundamental understanding of the mechanisms responsible for DDT in various settings.

High-speed turbulent deflagration, DDT, and resulting detonation waves present a significant hazard in the production and delivery of combustible chemicals and fuels. Hydrogen fuel is particularly sensitive to detonation, and DDT hazard is also a potential threat to the safety of nuclear reactors.

Because multiple effects and mechanisms may act concurrently on a DDT event, it is extremely difficult to obtain temporally and spatially resolved experimental DDT data. Detonation occurs quickly and on a very small spatial scale compared to the size of the system, making high-resolution, multidimensional simulations the most feasible method by which to investigate a detailed physics of DDT.

This study requires first-principles, compressible, reactive flow Navier-Stokes DNS, which take into account and explicitly resolve physical processes on spatial scales ranging from meters to microns, as well as attendant shocks, discontinuities, and physical variables.

Much of the current work on this project has been accomplished by using a high-speed combustion and simulation code on Mira. The code incorporates detailed physics and chemistry suitable for hydrogen combustion and high-resolution treatment of shock waves, and supplies a uniform grid as well as static and dynamic adaptive mesh refinement capabilities.

Researchers have conducted the first 3D reactive flow Navier-Stokes DNS simulations of flame acceleration and DDT in a stoichiometric hydrogen-oxygen mixture at 1 atm. initial pressure, in a 2.5 cm square pipe with smooth and rough walls. Wall roughness introduces additional turbulence which leads to a somewhat faster DDT and a drastic change in the location of the DDT from pre-heated gas ahead of the flame brush to hot spots inside it. Both modes of DDT have been experimentally observed in long tubes.

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INCITE | 200 Million Core-Hours

## Solving Petascale Public Health and Safety Problems Using Uintah

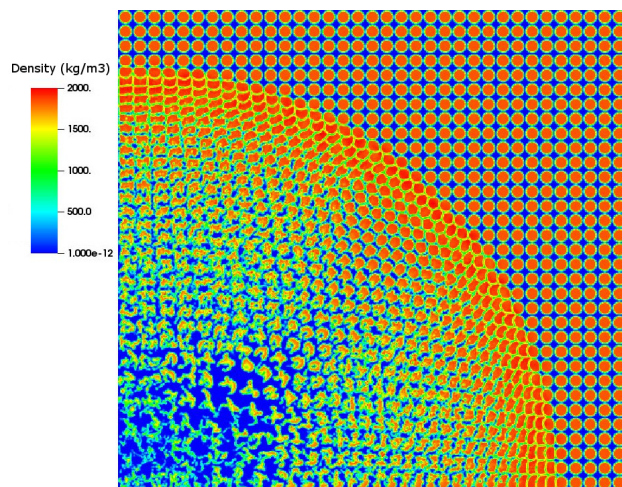
In 2005, a tractor-trailer rollover in Utah set off 36,000 pounds of high explosives that rapidly transitioned from an ordinary thermal explosion to a fully developed detonation, destroying a substantial section of highway and adjacent railway. To help improve the safe transport of explosives, researchers from the University of Utah are using Mira to examine how different packing arrangements and storage techniques can be used to stop such transitions.

The research team is using an INCITE allocation to run simulations to better understand the mechanisms of large-scale deflagration-to-detonation transition (DDT) of packed explosives. With the petascale power of Mira, they are able to perform simulations of sufficiently high spatial and temporal resolution to examine the impact of various explosive packing densities and configurations on DDT.

For one study, the team is investigating the reflection and coalescences of pressure waves in partially burned explosives. Thus far, they have found that the pressure waves did not amplify as a function of mass burned, as was originally hypothesized. The researchers are also working to determine how the pressure waves can transition into DDT and what other mechanisms could be responsible, depending on the geometry of the explosives and the packaging configuration.

In addition, the team has performed a large parametric study with simulations using 5,120 explosive cylinders to look at how packing density and spacing impacts the time to detonation. Preliminary results suggest a critical packing density of 40 percent for explosive cylinders with a radius of 0.027 m (the same radius as the cylinders involved in the 2005 truck accident). This means that if explosive cylinders are evenly spaced and occupy less than 40 percent of a container, they will not transition into detonation. The team continues to investigate how the cylinder radius impacts this critical packing density.

This work coincides with an ongoing National Science Foundation PetaApps project aimed at using simulation science to explore ways to use the Uintah computational framework to solve problems in public health and public safety. Uintah is a set of software components and libraries that facilitate the solution of partial differential equations on structured adaptive mesh refinement grids using hundreds to thousands of processors.



*Proposed DDT mechanism of inertial confinement. This image shows the density of the explosive cylinders late into the simulation.*

Image credit: Jacqueline Beckvermit, University of Utah

### IMPACT

**By providing a better understanding of the DDT process and potential mitigation strategies, this project stands to improve the safe storage and transport of explosive devices, which will ultimately improve the safety of our roads and railways. Additionally, the project is showing that it is possible to create the software needed to tackle such complex multiscale, multiphysics simulations with leadership-class supercomputers like Mira.**



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INCITE | 86 Million Core-Hours

## Upscaling Laws in Premixed Explosions

As fire propagates in an enclosed space, it heats the surrounding environment, creating an internal pressure that can build very rapidly and explode in dramatic fashion. Researchers from the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) are leading an international effort to better understand the mechanics of flame and explosion propagation, from the early laminar flame phase to the more aggressive turbulent flames that can incite explosion.

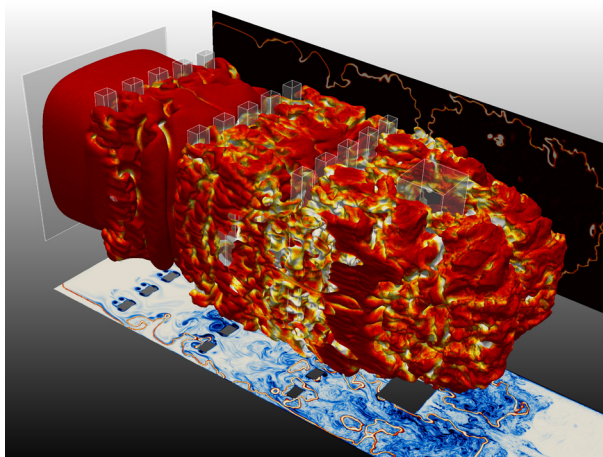
CERFACS researchers have worked closely with ALCF in the development of high-fidelity tools to simulate realistic explosion scenarios. Experiments conducted in Australia and Norway used dedicated chambers outfitted with baffles and columns to simulate obstacles in an enclosed space, and explosions were produced using premixed flame mixtures of propane and air. Information from the Australian experiment, derived from a small laboratory explosion in a vessel of 0.25 m, was used to upscale the Norway models to 1.5 m and 6 m.

The explosions were monitored using particle image velocimetry to track how minute particles introduced into the scenario move with the flame front. The propagation speed of the flame was measured at 40 cm/s to 250 m/s from start to finish, respectively. Vessel pressure was also monitored for an overpressure situation, which can cause the vessel to explode.

Working with ALCF personnel and the massive computing power of Mira, this data was then converted into the first-ever large eddy simulation (LES) of a building explosion. Contrary to previous computations, the present simulation correctly reproduces the timing and the amplitude of the explosion, due mainly to the introduction of a very fine grid comprised of 962 million tetrahedral elements, or nearly one-billion cells. At this resolution, predicting sub grid flame/turbulence interaction via a dynamic combustion model is greatly improved.

A combination of ParMETIS/METIS software was used to partition the grid and AVBP code was used to solve the 3D Navier-Stokes equations for reactive compressible two-phase flows on unstructured grids using the LES approach.

The simulations, thus far, have come close to capturing experimental trends, taking researchers one step closer to recreating real systems. Computational scientists at CERFACS and ALCF continue to work toward optimizing resolution at these larger scales.



*LES of an explosion in a venting chamber: instantaneous flame position (red isosurface), isocontour of reaction rate in a plane (back picture), turbulent viscosity field (bottom picture).*

Image credit: David Barré, CERFACS

### IMPACT

**These computer simulations have helped develop the world's largest database on turbulent flames to calculate peak pressures in an enclosed environment given a certain geometry and chemical composition of a flame front. This information will lead to the employment of better safety mechanisms and regulations, both in buildings and on offshore oil platforms.**

## Vibrational and Optical Spectroscopy of Electrolyte/Solid Interfaces

Photoelectrochemical (PEC) energy conversion is a promising approach to hydrogen production that uses solar energy to split water into hydrogen and oxygen gases. To help accelerate research and development efforts in this area, scientists from the University of Chicago and the University of California (UC), Davis, are using Mira to provide knowledge and build novel computational tools that can be used to better understand PEC processes at the microscopic scale.

One of the key challenges to developing scalable, commercially viable PEC cells is identifying stable and efficient photoelectrode materials. For this INCITE project, the research team is carrying out large-scale simulations at the ALCF to model the physical and chemical processes occurring at the interface between solid photoelectrodes and electrolytes. The simulation results can be used to create design rules that help predict the optimal photoelectrode materials to use for PEC water splitting.

To enable these studies, the researchers developed a set of simulation codes to probe and predict vibrational and electronic properties of the solid-liquid interfaces. In particular, they substantially improved the performance, scaling, and parallelization of Qbox (a first-principles, molecular dynamics code developed at UC Davis) on Mira. The Qbox development team also added modules to compute Raman and surface sensitive sum frequency generation spectra, including hybrid density functionals.

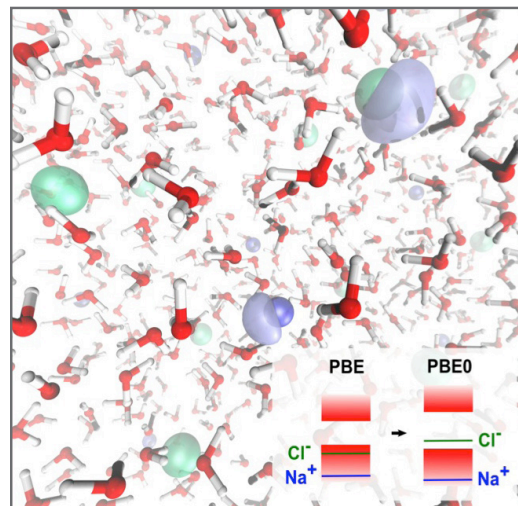
The use of functionals allowed the researchers to calculate the electronic properties of electrolytes, a challenging task for *ab initio* simulations. This computational approach, applied to both sodium chloride and sulfuric acid in water, takes full advantage of the massively parallel capabilities of Mira.

The team also developed algorithms and codes to enable first-principles calculations of the electronic properties of complex surfaces and interfaces within many-body perturbation theory at the GW level, enabling GW calculations of unprecedented size for slabs containing solid-liquid interfaces. Although this INCITE project is focused on PEC, the methodologies and results stemming from this work are relevant to other energy-related research efforts, including electrical energy storage and solar cells.

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INCITE | 70 Million Core-Hours



Snapshot of a 1 M solution of NaCl obtained from an *ab initio* molecular dynamics simulation with a hybrid (PBE0) functional. Red, white, purple, and green spheres represent oxygen, hydrogen, sodium, and chlorine atoms, respectively. The electronic properties of  $[\text{NaCl}]_{\text{aq}}$ , computed with PBE0 and semi-local (PBE) functionals, are shown in the right corner of the figure.

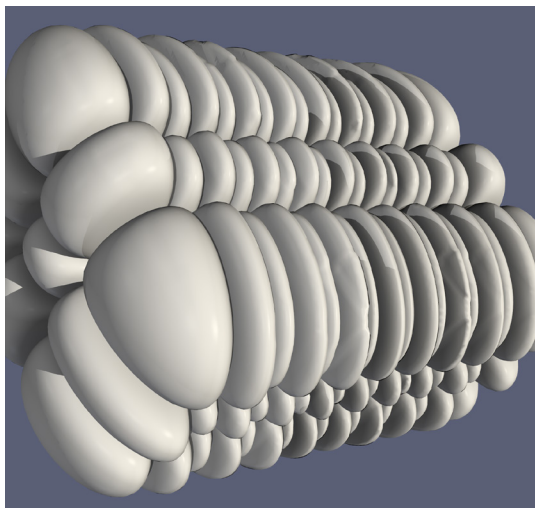
Image credit: Alex Gaiduk, University of Chicago

### IMPACT

**This project is providing knowledge and computational tools to interpret and inform ongoing experiments on hydrogen production from water. The results can be used to establish design rules to predict materials optimally suited to reduce and oxidize water, which could ultimately help accelerate the development of technologies for sustainable and clean hydrogen production.**

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INCITE | 20 Million Core-Hours



*A neutron wave-function for a benchmark calculation using a Skyrme functional for the Hartree-Fock-Bogoliubov equation in nuclear physics is solved using an extension of MADNESS, MADNESS-HFB, in coordinate space.*

Image credit: George Fann,  
Oak Ridge National Laboratory

## Dynamic and Adaptive Parallel Programming for Exascale Research

The path from petascale to exascale computing poses many challenges for hardware architectures, system software developers, and application programmers. This project will continue R&D activities into the design, development, deployment, and demonstration of a novel programming environment that addresses both the programming model and algorithmic challenges of exascale computing within multiple domains.

This project supports the very active community developing and employing high-performance and high-productivity parallel programming paradigms that provide a natural and fully compatible extension of the message passing interface (MPI) to massively threaded, extreme-scale parallel systems. The computer science and math research will bring a broad suite of science applications closer to exascale readiness.

The application domains targeted for demonstration include nuclear physics, density functional theory (DFT) of materials, and quantum many-body methods for chemistry. The experiment apparatus will be the MADNESS framework, which encapsulates a dynamic active-message runtime system, a global data model based upon distributed containers, a multiresolution analysis (MRA) toolkit, and scalable numerical solvers.

Early work on Mira included the development of high-performance kernels using code generation/transformation with polyhedral analysis and autotuning. Threading Build Blocks has also been tested with the aim of replacing MADNESS' own thread runtime to improve the asynchronous parallelism and improve load balance within a work-stealing approach. In addition, work has been done to improve the performance of distributed tensor contractions, with scalability demonstrated up to 16,384 nodes.

Recent work for the DFT code has included the implementation of pseudopotentials, which reduce the number of electrons that are explicitly treated and therefore decrease the cost of molecular simulations. Work is ongoing to integrate a newly implemented approach to calculating inner products in MADNESS.

Ease of parallel programming based on object-oriented abstractions hiding low-level message passing, optimization of distributed multicore performance, and the applications of multiresolution mathematical operations has enabled the rapid development of an extensible and scalable framework for solving many-body systems and density functional theory for nuclear structures. MADNESS's programming models and its extensions are designed to solve larger complex nuclear physics problems for exascale systems.

### IMPACT

**This project will provide a refined understanding of massively threaded scalar/vector programming models with experience at full system scale in complete and diverse science applications; preparation of the parallel runtime and associated science applications for the interim exascale systems; new science application functionality; and unification of intra-node multi-/many-core/hybrid programming models within MADNESS.**

### LEONID OLIKER

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 INCITE | 75 Million Core-Hours  
 ALCF 30 Million; OLCF 45 Million

## Performance Evaluation and Analysis Consortium (PEAC) End Station

The DOE Office of Science has made a substantial investment in its leadership-class computing systems. Through a collaboration of researchers from leading national laboratories, the Performance Evaluation and Analysis Consortium (PEAC) End Station was established to engage its members in research to maximize the utility, efficiency, and effectiveness of these systems.

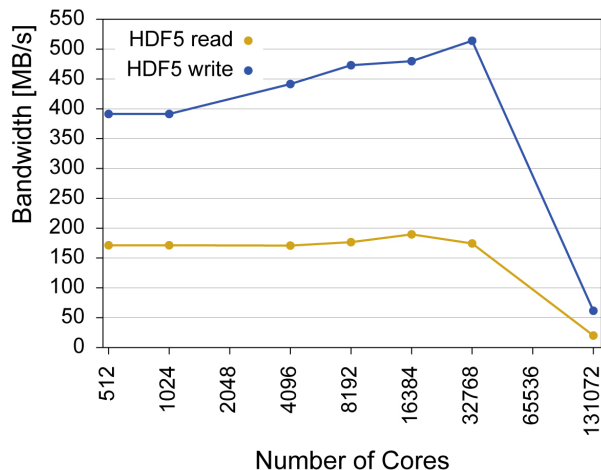
PEAC provides a mechanism for the computer science community to contribute to the success of leadership-class systems and the scientific results generated by them, independent of project size or hour allocation.

The PEAC community leverages DOE leadership computing resources to make substantial contributions to the understanding of these systems in five key areas: (1) development of new programming models and runtime systems; (2) enhanced performance evaluation of new and emerging systems; (3) development and porting of performance tools and performance middleware to support the scale and unique modes of parallelism; (4) validation and modification of performance prediction technologies, and; (5) analysis and optimization of current or candidate application codes.

PEAC consortium members have an established track record of effective interaction with computational science teams, which has led to significant performance improvements in numerous important application codes.

Key recent contributions on ALCF resources include the scalability of the Cyclops Tensor contraction framework by University of California researchers. This has allowed PEAC team members to perform the largest coupled-cluster (CC) calculation to date: namely CCSD (single and double excitations) with 250 electrons with over 1000 orbitals, and CCSD(T) (triple excitation) with 55 electrons and 250 orbitals.

Mira was also used to evaluate and benchmark the performance of the new HDF5-based QDP++ I/O library developed by Lawrence Berkeley National Laboratory team members. This library, part of the Lattice Quantum Chromodynamics (LQCD) software stack, eases I/O usage in LQCD codes, providing highly stable and consistent performance regardless of the problem size or I/O geometries used.



*New parallel HDF5-based I/O implementation in the Lattice QCD software stack (QDP++) improves existing QIO library performance by an average of 50 percent.*

Image credit: Abhinav Sarje, et al., Lawrence Berkeley National Laboratory

### IMPACT

**Access to these unprecedented concurrent and heterogeneous systems will make it possible to effectively conduct research into platform specifics that will support computational science and assist scientists in maximizing the speed and, therefore, the impact of these large-scale systems.**

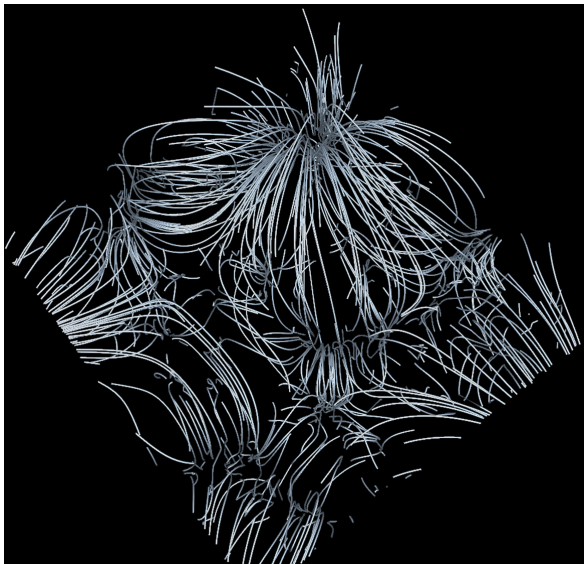


### ROBERT LATHAM

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INCITE | 25 Million Core-Hours



*Streamlines from an early time step of the Rayleigh-Taylor instability depend on scalable storage, communication, and data analysis algorithms developed at extreme scale using INCITE resources.*

Image credit: Tom Peterka,  
Argonne National Laboratory

### IMPACT

**Work done through SSSPP will allow computational scientists to simultaneously achieve performance and productivity on extreme-scale systems by effectively allowing applications to utilize the processing, communication, and storage capabilities hidden under the architectural complexity of leadership-class computers.**

## Scalable System Software for Parallel Programming

Computational scientists face ever greater challenges in terms of parallelism and performance maximization with each generation of leadership-class computing systems. The Scalable System Software for Parallel Programming (SSSPP) project aims to mitigate that challenge by developing algorithms, abstractions, and libraries to provide maximum computational performance, while allowing computational scientists to ignore some of the lower-level details.

An Argonne research team is working with IBM to explore ways to make the existing Blue Gene/Q software environment more productive for computational scientists. The SSSPP project is addressing three areas: programming models, high-performance I/O, and analysis.

The researchers have identified several faults and ways to improve the message passing interface (MPI) library installed on the Blue Gene/Q series of machines. For example, by adjusting the default tuning parameters for I/O and the algorithms behind several MPI routines, certain applications can now scale to large fractions of the machine. While not officially supported by IBM, a “community edition” of the Blue Gene MPI library will provide MPI-3 features, improved I/O performance, and better scalability for several important MPI routines.

The Argonne team also developed a new parallel algorithm for computing Delaunay and Voronoi tessellations, which convert discrete point data into a continuous field. The primary challenge was to automatically determine the points to exchange among neighboring blocks in order to form the correct global tessellation.

The results showed that the algorithms produce the correct result provided that all Delaunay edges fit within a one-neighborhood of blocks, where the block size is larger than the interparticle spacing. It also proved that, despite the networking speed of today’s high-performance computers, all communication can be determined locally. This approach suggests that answers can be more readily accessed, and computing resources can produce more science.

**MARK TAYLOR**

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INCITE | 150 Million Core-Hours  
ALCF 50 Million; OLCF 100 Million

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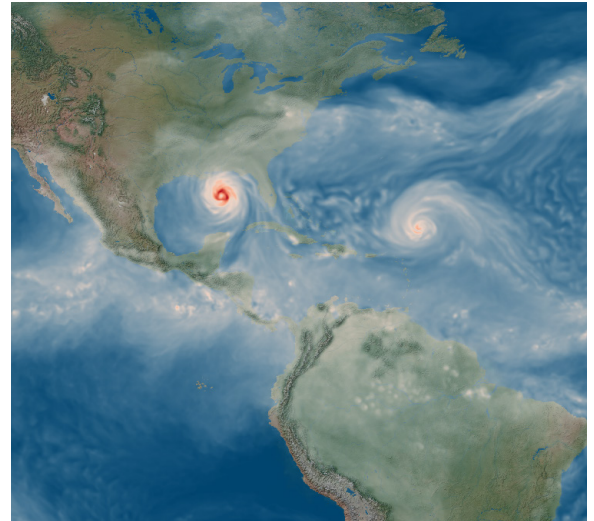
## High-Resolution Simulation for Climate Means, Variability, and Extreme

In the next few decades, the frequency and intensity of extreme weather events is expected to increase along with global greenhouse gas emissions. Improved climate models are needed to better understand and predict extreme weather events, such as storms, droughts, and floods. This INCITE project aims to improve the Community Earth System Model (CESM) by using DOE supercomputers to employ new model configurations at very high resolution.

A team of researchers from several national laboratories is scaling CESM, a global climate model jointly supported by DOE and the National Science Foundation, to run on leadership computing resources to improve the modeling of climate change and its impact on extreme events at the regional scale. To enhance these capabilities, very high resolution is required, as well as improvements to many other aspects of the model, such as the subgrid parameterizations of unresolved physical processes.

The researchers are developing an atmospheric testbed that uses novel methods to achieve the resolution necessary to test and improve parameterizations. The testbed combines CESM's new regional refinement capability, modern uncertainty quantification methods, and extensive observational datasets collected at the DOE's Atmospheric Radiation Measurement (ARM) sites. Regional refinement allows the team to examine a small region in very high resolution and transitions the rest of the globe to low resolution. This technique, combined with the petascale power of Mira, makes it possible to run the hundreds of simulations necessary to develop and calibrate parameterizations suitable for high-resolution climate modeling.

Thus far, the team has completed the first regionally refined simulations, with refinement down to a 13 km resolution over the ARM Southern Great Plains site. The team has also completed a five-year simulation with globally uniform 13 km resolution, which will be used to verify the regionally refined simulations and to establish a baseline of the quality of the simulations produced by the existing CESM at 13 km resolution.



*An example of a Category 5 hurricane simulated by the CESM at 13 km resolution. Precipitable water (grey scale) shows the detailed dynamical structure in the flow. Strong precipitation is overlaid in red. High resolution is necessary to simulate reasonable numbers of tropical cyclones including Category 4 and 5 storms.*

Image credit: Alan Scott and Mark Taylor, Sandia National Laboratories

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### IMPACT

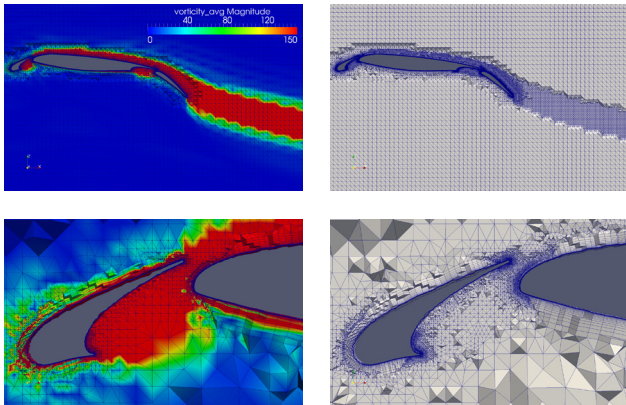
**This project is using DOE supercomputers to improve the CESM by employing new model configurations with very high resolution. The enhanced climate model will provide a better understanding of how extreme weather is impacted by climate change, which will ultimately improve our ability to plan for severe weather events.**

**KENNETH JANSEN**

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INCITE | 66 Million Core-Hours



*Illustration of mesh adaptation with a slice through the mesh of a three element high lift wing (three element view for top images; slat and main wing view for bottom images). The elements highlighted in red in the initial mesh are adapted based on their high value of mean vorticity magnitude. The initial mesh in the left images includes 895 million elements and the adapted mesh in the right images include 1.3 billion elements.*

Image credit: Kenneth Jansen,  
University of Colorado

## Adaptive Detached Eddy Simulation of a High Lift Wing with Active Flow Control

Recent developments in parallel adaptive meshing and parallel solver technology are yielding fundamental insight into the complicated physics of flow control on real aircraft configurations. Using these techniques, project researchers are modeling an array of synthetic jets that have been specifically vectored to improve the aerodynamic performance of wing profiles in aeronautics.

The goal of aerodynamics is to improve vehicle performance over a wide range of operating conditions. Traditionally, this has been done with mechanical flaps, but an alternative approach is to employ active flow control using synthetic jet actuators.

Active flow control can alter a natural flow field into a more desirable state when synthetic jet actuators are placed at key locations along an aircraft wing in order to improve efficiency and performance. This can prevent or reduce flow separation, which limits flap effectiveness for high-deflection angles.

Complementing previous INCITE and Early Science Program research, this project applies more advanced turbulence models which resolve, rather than model, the energetic turbulent eddies that accompany very complicated high lift, aerodynamic geometries, such as multi-element wings. Slats and flaps are deployed for landing configurations and their performance limit is dictated by flow separation. Project simulations model this limit to higher performance through the use of active flow control.

Simulations of the high lift configuration at two different angles of attack have been completed with both base turbulence and higher-fidelity turbulence models. Also, researchers have adapted the meshes to confirm regions where solutions will not change with further mesh refinement and identified regions that can benefit from adaptation.

The computational approach used for these simulations is the finite-element based flow solver, PHASTA, employed with anisotropic adaptive meshing and partitioning procedures. The results were processed on Tukey, the ALCF's visualization cluster. This enabled the distillation of multi-terabyte datasets to a level that allows researchers to compare the overall performance of the wing to detailed experimental results. Full surface and volume data have also been visualized to better understand the fundamental flow physics.

### IMPACT

**Research on the high lift wing configuration can help improve aircraft designs and increase fuel efficiency by reducing aircraft weight and drag. Fuel costs, which are now the dominant cost in passenger air travel, can be substantially reduced, and side benefits may include longer flight range.**

## LEE SHUNN

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INCITE | 100 Million Core-Hours

## Combustion Stability in Complex Engineering Flows

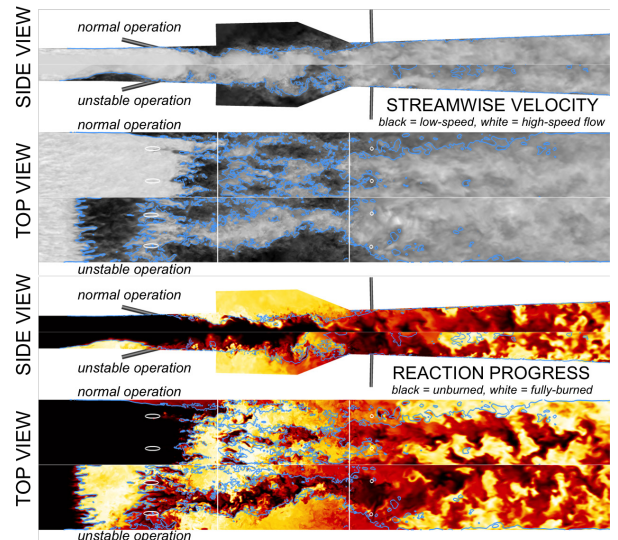
Combustion instabilities can negatively impact safety and efficiency in a wide range of combustion systems, including rocket motors, scramjets, furnaces, and power plants. For this INCITE project, scientists from Cascade Technologies and GE Power & Water are using Mira to simulate combustion instabilities in real-world applications to better understand why they occur and how to prevent and control them.

Complex interactions between chemistry, turbulence, and acoustics can destabilize combustion systems and lead to intense pressure fluctuations and heat transfer. These instabilities complicate operations and, in some cases, result in structural damage to equipment and facilities. Experimental methods can shed some light on the growth and propagation of unstable combustion processes, but improved predictive capabilities are needed to mitigate them in real engineering devices. With this INCITE project, the research team is working to develop efficient and scalable numerical methods to predict unsteady combustion in gas turbine engines and scramjets.

For the turbine study, the team is modeling a GE Dry Low-NOx (DLN) combustor used in land-based gas turbines.

In DLN engines, the dual constraints of low emissions and safe operations present competing trade-offs to maintaining stable combustion in lean, partially premixed regimes. For the scramjet simulations, the researchers are looking at high-speed engines from the Hypersonic International Flight Research Experimentation (HIFiRE) program. An earlier NASA report compared the challenge of stabilizing combustion in scramjet engines to “keeping a match lit in a hurricane.”

To numerically reproduce combustion instabilities in these challenging environments, the team is performing simulations on Mira using CharLES, the unstructured large eddy simulation solver developed and licensed by Cascade Technologies. CharLES provides unique low-dissipation numerics, dynamic turbulence models, and massive scalability to enable these problems to be studied under realistic operating conditions in complex engineering geometries. In addition to predicting engine-level stability, the simulations are being used to characterize operability limits, emissions, and reliability/durability in the target applications.



Separation and reverse flow cause large-scale disruptions in the HIFiRE scramjet. During the instability, pockets of combustion anchor in the low-speed regions (colored dark in the grayscale image) upstream of the fuel injectors and along the sidewalls. The blue line indicates the division between subsonic and supersonic flow.

Image credit: Lee Shunn, Cascade Technologies

## IMPACT

**Simulations from this project are providing a better understanding of instabilities in applied combustion systems. The detailed numerical results are being used to assess combustion system performance and evaluate prediction tools commonly used by design engineers. Ultimately, this research will advance the development of safer and more efficient propulsion and industrial combustion systems.**

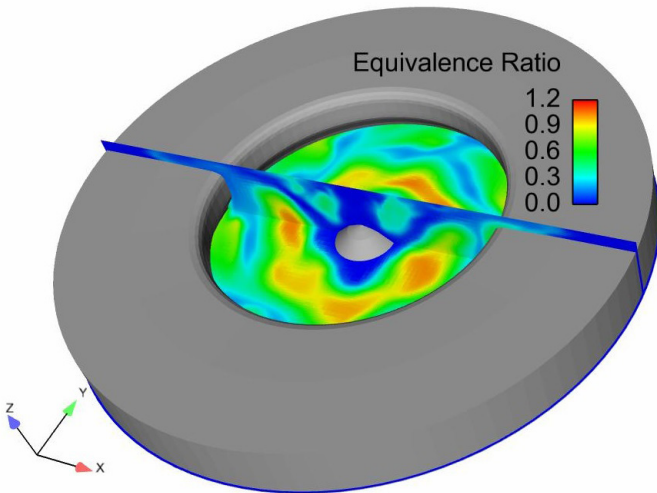


**SIBENDU SOM**

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Director's Discretionary | 1.5 Million Core-Hours



*This figure shows the equivalence ratio distribution within the engine piston bowl during combustion for an advanced engine concept called gasoline compression ignition (GCI). Argonne researchers attempt to control GCI combustion based on equivalence ratio distribution.*

Image credit: Janardhan Kodavasal,  
Argonne National Laboratory

## Development of Predictive Multidimensional Combustion Modeling Capability with Detailed Chemistry

As an alternative to traditional “build and test” engine design processes, automotive and engine manufacturers are becoming increasingly reliant on computers to aid in the design of next-generation engines. With a Director’s Discretionary (DD) allocation at the ALCF, Argonne researchers are using supercomputers to develop more powerful modeling and simulation capabilities to shed new light on the complex processes taking place inside combustion engines.

With the ability to optimize complex fuel spray and combustion processes for a variety of fuels over a wide range of operating conditions, engine modeling and simulation tools can help manufacturers improve engine efficiency and performance, while reducing development costs and accelerating time to market.

As part of a Laboratory Directed Research and Development project at Argonne, a multidisciplinary team of researchers is working to develop a multidimensional combustion modeling capability for automotive engine applications. Their efforts have led to the creation of Argonne’s Virtual Engine Research Institute and Fuels Initiative (VERIFI), a new platform for industry collaboration that leverages the laboratory’s expertise and tools in high-performance computing, fuel chemistry, combustion science, and engine performance.

The researchers are currently using a DD allocation at the ALCF to optimize and improve the scalability of the CONVERGE code, a computational fluid dynamics software program widely used by industry, on high-performance computers. Working closely with ALCF staff, the team initially focused on improving the I/O performance of the CONVERGE solver. To do so, they tested two cases: a small case with a 20,000-cell grid and a larger case with a 35-million-cell grid. In both cases, the researchers observed that I/O performance was mainly driven by the time required to write the output for post-processing visualization and the restart files. To speed the writing time scales, they reduced the number of calls to the *fwrite* function by storing the variables in arrays. This led to a factor-of-24 improvement for the write time of the output files and an overall I/O performance improvement of a factor of four. In preparation for a more substantial allocation at the ALCF, the team continues work to optimize the code to take full advantage of Mira’s petascale power.

### IMPACT

**This project aims to develop novel engine modeling and simulation capabilities for high-performance computers, providing automotive manufacturers with a cost-effective tool to accelerate the development of more energy-efficient engines. Ultimately, these tools have the potential to improve the fuel economy of vehicles, thereby reducing U.S. dependence on foreign oil and reducing carbon emissions.**

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ALCC | 11 Million Core-Hours

## Does a Turbulent Duct Flow Ever Become Two-Dimensional?

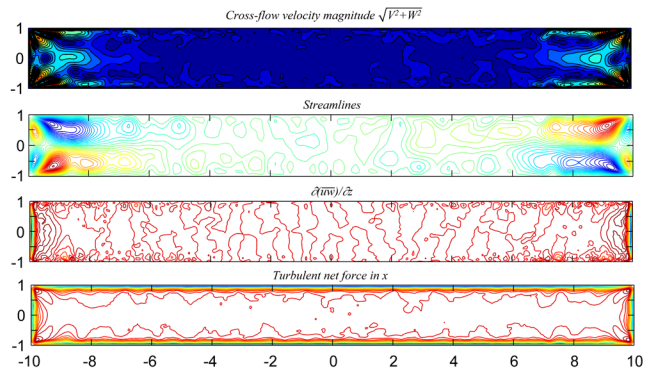
Globally, about 10 percent of energy consumption is used to overcome turbulent drag in one way or another. Numerous real-world applications involve the flow of fluid through a rectangular duct, including urban drainage systems, ventilation systems, and combustion engines. Through simulations at the ALCF, researchers are working to better understand turbulent flow physics in rectangular ducts with the goal of enabling new methods to reduce drag and friction.

Traditional computational studies of turbulent flow within a duct have always assumed that if the duct is wide enough, it can be treated as infinitely wide (2D, or z-periodic). However, recent experiments performed by researchers at the Illinois Institute of Technology (IIT) showed that this 2D assumption is not representative of the physical flow for many realistic flow regimes.

The IIT research team, in collaboration with researchers at KTH Mechanics, in Sweden, then received an ALCC allocation to study the results of their experimental measurements. Using ALCF supercomputers, they ran simulations with the highly scalable Nek5000 code to examine the behavior of turbulent flow through rectangular ducts for increasing aspect ratios (ratio of width/length) and more realistic Reynolds numbers.

The team examined several duct aspect ratios, which led to some interesting physical conclusions. At higher aspect ratios (ranging from 12.8 to 48), the calculated skin friction decreased as the aspect ratio increased up to 24, where it then appeared to reach an asymptotic value. Computations of ducts with aspect ratios from 1 to 10 revealed that increasing the aspect ratio from 1 to 3 actually increased the friction. The researchers determined this increased friction results from a complex relationship between the side-wall boundary layers and secondary motions in the flow. These secondary motions significantly impact the overall flow physics but have not been documented in the literature because they are extremely difficult to detect in the laboratory.

The secondary vortices and side-wall boundary layers have been studied in detail, as well as their evolution with increased Reynolds numbers and aspect ratios. The results provide justification for the computational fluid dynamics community to redirect efforts from studying flows that have no counterpart in real life, such as the z-periodic channel, to more relevant wall-bounded and ducted flows.



Streamwise- and time-averaged statistics of turbulent duct flow (with aspect ratio 10) computed at  $Re_{\tau}$  of 180.

Image credit: Paul Fischer and Aleksander Obabko, Argonne National Laboratory; Hassan Nagib, Illinois Institute of Technology; Ricardo Vinuesa, Illinois Institute of Technology/KTH Royal Institute of Technology; Philipp Schlatter, KTH Royal Institute of Technology.

### IMPACT

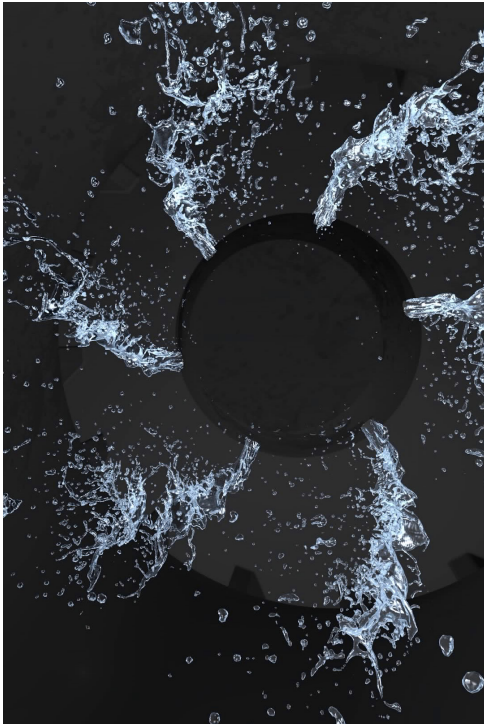
The simulations from this project have shed light on the existence of important fluid flow physics that have been postulated but difficult to observe in the laboratory. The results will feed into the development of more accurate turbulence models, which will help enable the discovery of new methods to reduce drag and skin friction for a variety of applications.

**PARVIZ MOIN**

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ALCC | 150 Million Core-Hours



*Swirl injector for a gas turbine combustor showing the breakup and atomization of six liquid fuel streams in a high-shear airflow.*

Image credit: Dokyun Kim, Cascade Technologies, Inc.

### IMPACT

**This project is demonstrating the potential of LES and high-performance computing as a powerful, yet cost-effective design tool for practical engineering flows. By providing a better understanding of turbulence and its impact, computational tools like CharLES can help industry advance the design and optimization of more energy-efficient technologies, such as airplanes, automobiles, fuel injectors, and turbines.**

## Wall Modeling and Primary Atomization for Predictive Large Eddy Simulation of Airframes, Jet Engines, and Jet Noise

Large eddy simulation (LES), a mathematical model used to predict turbulence, is emerging as an accurate yet cost-effective computational tool to aid in the design of more energy-efficient engineering systems, such as airplanes, automobiles, and turbines. Researchers from Stanford University are using ALCF supercomputers to develop and demonstrate high-fidelity LES methods that could be used by industry to advance aviation, transportation, and clean energy technologies.

With this ALCC project, the Stanford research team aims to validate several novel LES models for near-wall turbulence, fuel atomization, and reacting flows in an unstructured grid environment implemented in the CharLES code framework developed at Cascade Technologies. To perform the simulations, they worked with ALCF staff to optimize sparse-matrix-vector multiplication, partitioning, and large-mesh support in CharLES, which more than doubled the code's speed. This enabled the research team to move forward with three case studies that stressed new LES capabilities.

First, they performed LES of the turbulent reacting flow inside the HIFiRE-2 scramjet engine. The integrated simulations employed the CharLESx unstructured, compressible flow solver leveraging several advances in wall modeling, flamelet modeling, turbulent inflow generation, and shock-capturing schemes that minimize numerical dissipation. The team generated a comprehensive numerical database and validated it against ground tests with unprecedented agreement.

For the second case study, the researchers used a novel LES wall model to study automotive side-view mirrors, a dominant source of noise in electric vehicles. To mitigate mirror noise, engineers need an accurate prediction of the transition location and separated flow region. The Stanford team's slip-based wall model, which dynamically treats laminar to turbulent transition without ad-hoc sensors, was consistently validated with experimental data from Honda's wind tunnel and shown to dynamically compute transition across all flow regimes.

Finally, the researchers examined the atomization of kerosene jet fuel in a complex geometry swirling injector with six liquid jet inlets. The simulations were performed using a volume-of-fluid method coupled with a Lagrangian particle-tracking approach for secondary droplet breakup implemented entirely on unstructured grids.

**JEFFREY GREELEY**

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 ALCC | 75 Million Core-Hours  
 ALCF 50 Million; OLCF 25 Million

## First-Principles Investigations of Adsorbate-Metal Interactions: Quantum Monte Carlo and Ab Initio Molecular Dynamics Simulations

The chemical reactions and catalysis that occur at the interfaces between metal surfaces and aqueous environments are ubiquitous in fuel cells, electrolyzers, and a variety of chemical processes relevant to the biomass and petrochemicals industries. The broad goal of this project is to develop more realistic computational descriptions of how molecules bind to metal surfaces.

Researchers at Purdue University and Oak Ridge National Laboratory are using highly accurate electronic structure calculations, known as quantum Monte Carlo (QMC) simulations, to achieve a greater level of accuracy of molecular binding than has been achieved for metal surfaces. In addition, a combination of electronic structure and *ab initio* molecular dynamics (AIMD) simulations are being used to better understand how the molecules move on specific surfaces.

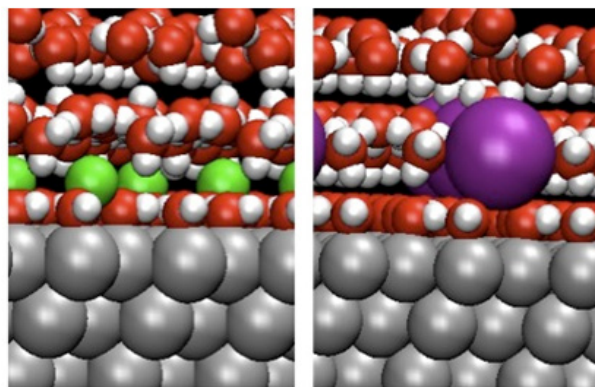
Many of these molecules interact with metal surfaces through weak Van der Waals forces, electron lone pairs, or electron donation/back donation mechanisms, though standard density functional theory (DFT) calculations describe these interactions rather poorly.

This is one of the first studies to both improve the accuracy of standard DFT treatments of weak adsorbate-metal bonding and add finite-temperature dynamical effects to the analysis of water-metal interactions. The QMC calculations involved a combination of methods to determine the interaction energies of water layers, carbon monoxide molecules, and nitrogen-containing oxide molecules with single-crystal platinum (Pt) surfaces at an unprecedented level of accuracy.

A very accurate calculation was recently performed to determine the surface energy of a platinum crystal, using the QMCPACK code on Mira.

These surface energies are important in determining the shapes of platinum-based nanoparticle catalysts, and such surface energies are difficult to calculate with any accuracy using lower levels of electronic structure calculations.

Another aim of the study is to understand the complicated molecular, electronic, and electrostatic characteristics of the double layer, a fundamental structure in nearly all electrochemical systems. Difficult to study using even the most advanced experimental techniques, researchers are employing AIMD simulations to develop improved double layer models and explore their effect on the electroreduction chemistry of nitrogen-containing compounds on both Pt(111) and Pt(100) surfaces.



*Electronic structure simulations of solvated molecular and atomic species near Pt(111) transition metal surfaces.*

Image credit: Jeffrey Greeley, Purdue University

### IMPACT

**A primary goal of the proposed research is to develop highly accurate, fundamental models of electrochemical structures and processes and their effect on electrocatalytic reactions. These properties are relevant to a broad spectrum of electrochemical phenomena, from the performance of renewable fuel cells to the remediation of environmental pollutants.**

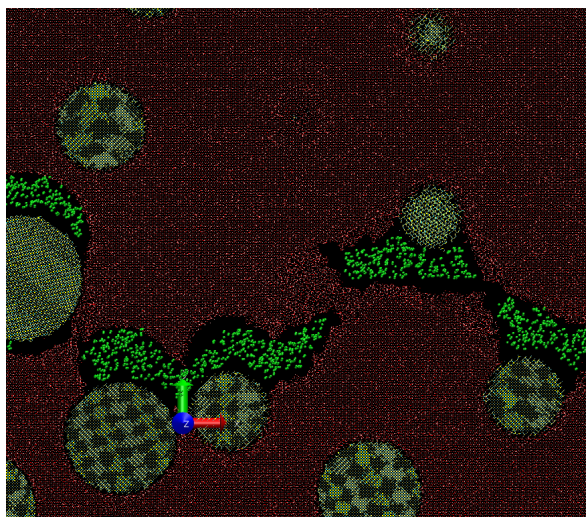


**RAJIV KALIA**

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INCITE | 200 Million Core-Hours



*Reactive molecular dynamics simulation to study the oxidation of fractured alumina matrix embedded with silicon carbide nanoparticles.*

Image credit: Rajiv Kalia, Ying Li, Aiichiro Nakano, Ken-ichi Nomura, Pankaj Rajak, and Priya Vashishta, University of Southern California

## Petascale Simulations of Self-Healing Nanomaterials

Self-healing nanomaterials are capable of sensing and repairing damage, such as cracks, in devices that operate in harsh conditions. With the ability to enhance reliability and reduce maintenance costs, these materials show great promise for use in energy technologies. Researchers from the University of Southern California (USC) are performing massive simulations on Mira to help advance the understanding and viability of self-healing nanomaterials.

The goal of the project is to determine the atomistic mechanisms underlying these remarkable self-healing capabilities. To do so, the USC research team is using ALCF resources to carry out quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and mesoscale simulations of two types of systems: (1) anticorrosion coatings for metals and (2) ceramic nanocomposites consisting of silicon carbide nanoparticles embedded in alumina and silicon nitride.

To prepare for the simulations, the team worked with ALCF staff to tune and debug their codes for optimized performance on Mira. The researchers also implemented an innovative divide-and-conquer density functional theory algorithm to enable QMD simulations of unprecedented scale. Their efforts have resulted in excellent weak-scaling and strong-scaling parallel efficiencies (0.984 and 0.803 on the full machine, respectively), improved time to solution (60 times faster than previous state-of-the-art calculations), and improved performance (from 30 percent to 50.5 percent of Mira's theoretical peak, or 5.1 petaflops). The team successfully used this code in a previous INCITE project at the ALCF to study hydrogen production from aluminum-water reactions. Those massive QMD simulations are helping the researchers advance their studies of anticorrosion coatings for metals.

For the ceramic nanocomposite work, they are looking at how the oxidation of silicon carbide at higher temperatures produces silicon dioxide, which can flow into cracks to heal them. The researchers are examining this phenomenon with RMD simulations of a 100-million-atom system consisting of a fractured alumina matrix embedded with silicon carbide nanoparticles.

The computational results from this project will be validated with data from experiments at DOE facilities, such as the Advanced Photon Source at Argonne National Laboratory, Spallation Neutron Source at Oak Ridge National Laboratory, and SLAC Linac Coherent Light Source at Stanford University.

### IMPACT

**This project will provide a fundamental understanding of self-healing nanomaterials, helping to accelerate the discovery of new materials for use in extreme conditions. Ultimately, this work could help enhance the reliability and reduce the cost of components for many energy applications, including high-temperature turbines, and wind and solar energy technologies.**

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INCITE | 100 Million Core-Hours

## Predictive Materials Modeling for Li-Air Battery Systems

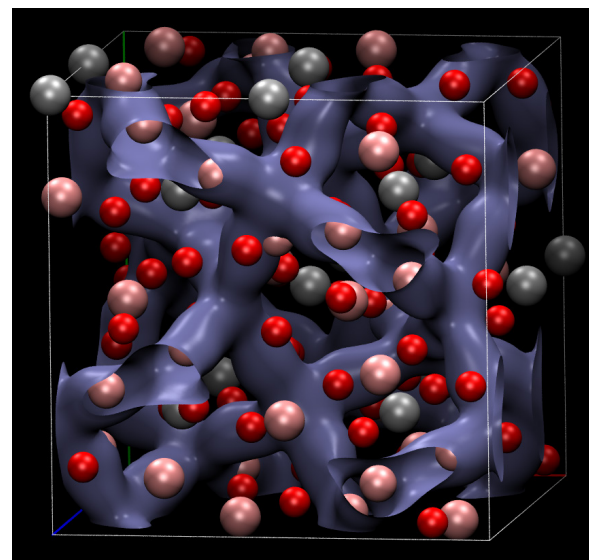
Lithium-air (Li-air) batteries are viewed as a possible game changer for electric vehicles, but realizing their enormous potential is a very challenging scientific problem that requires the development of new materials for electrodes and electrolytes. Scientists from Argonne and IBM Research are teaming up to use Mira to better understand the physical and chemical mechanisms needed to make Li-air batteries a reality.

With the potential to store up to 10 times the energy of a Li-ion battery of the same weight, Li-air batteries are particularly appealing to researchers because of their theoretical energy density. But developing a viable Li-air battery is a long-range effort that requires scientific breakthroughs in materials design, chemistry, and engineering.

One of the most significant hurdles is finding suitable materials for Li-ion-conducting electrolytes, which enable the transport of ions between the anode and the cathode and promote the diffusion of oxygen from the environment into the electrochemical cell. With this INCITE project, Argonne and IBM Research are conducting *ab initio* density functional theory (DFT) simulations on Mira to help accelerate efforts to identify novel materials for electrolytes.

In a recent study, IBM researchers focused on the zirconium-containing, garnet-like lithium-lanthanum-oxide, known as LLZO ( $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ ), a promising material for solid-state electrolytes. Experimental work has determined that the cubic phase of LLZO is much better at conducting Li-ions than its tetragonal phase, but computer simulations were required to investigate and compare the different mechanisms of Li-ion migration in the two phases.

To observe Li-ion migration, the team needed to simulate time scales in nanoseconds rather than picoseconds. They were able to achieve this factor-of-a-thousand improvement by implementing a highly efficient parallel version of metadynamics (a tool for accelerating rare events, such as mapping the conductivity of a material regardless of its complexity) into their DFT simulations and by taking advantage of Mira's substantial power with full machine runs. This enabled the researchers to obtain, for the first time, the free-energy profile for Li-ion conductivity in LLZO. One of their key findings was that the presence of vacancies in cubic LLZO is crucial to lowering its activation energy and enhancing its Li-ion conductivity.



An image of the LLZO material (200 atoms). The tubes depict iso-surface representations of the free-energy surface of Li-ion conductivity. Within the tubes, Li atoms (pink) can be observed moving inside the material.

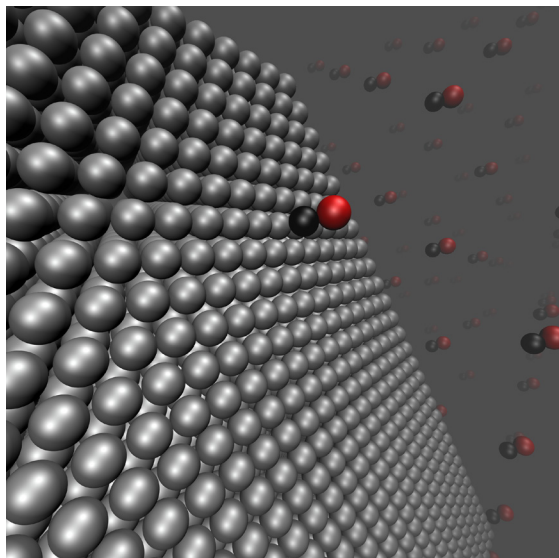
Image credit: Alessandro Curioni and Teodoro Laino, IBM Research Zurich

### IMPACT

This project is providing insight into the complexities of the Li-air battery at the molecular level, including an understanding of the microscopic mechanism for high Li-ion conductivity. The results will help to inform the design of new materials for Li-air electrolytes and electrodes. If realized, Li-air batteries could enable widespread deployment of electric vehicles, greatly reducing U.S. dependence on foreign oil.

### DAVID CEPERLEY

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INCITE | 200 Million Core-Hours  
ALCF 100 Million; OLCF 100 Million



*Carbon monoxide adsorbs on the Pt(111) surface. One application of this INCITE project is to model this important surface reaction which is poorly modeled by methods with static treatment of electron-electron interaction.*

Image credit: William Parker,  
Argonne National Laboratory

### 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 for applications, currently ranging from the simulation of materials in the interior of rocky and gaseous planets to catalysis of hydrocarbon reactions and surface chemistry.**

## QMC Simulations Database for Predictive Modeling and Theory

Quantum Monte Carlo (QMC) has the potential to make a significant impact in scientific areas where chemical accuracy (1 kilocalorie/mol) is required for realistic predictions of material properties. The scale of leadership computing resources lends itself well to a suite of QMC methods, which are naturally massively parallel algorithms. This project is part of a larger collaborative effort to harmonize and systematize QMC research across multiple U.S. institutions and national laboratories.

QMC encompasses a suite of accurate methods to simulate electron-electron and electron-nuclear interactions and provides a uniform way to treat electrons under vastly different physical conditions. Unlike many other electronic structure methods, QMC employs explicitly correlated wave functions to dynamically describe many-body effects, allowing QMC, in principle, to address a much broader range of materials phenomena. To this end, QMC utilizes stochastic processes to moderate the solution of electron and nuclei in full quantum mechanical terms.

This project brings together disparate efforts using continuum-based QMC to model electronic structure and light nuclear-electronic systems, calculating properties that emerge from these utilizing the QMCPACK program ported on Mira. Project researchers are studying heterogeneous catalysis of transition metal nanoparticles, phase transitions, properties of materials under pressure, and strongly correlated materials.

Recent work derived from this research has accurately modeled a transition between the crystal structures of magnesium silicate, a major Earth mineral believed to be responsible for unusual seismic wave modulations that occur at the core-mantle boundary. Additionally, QMC calculations of the continuous transition of hydrogen under pressure from molecular to monatomic fluid produced a relationship directly measurable by and therefore comparable to shock-wave experiments.

Investigation into platinum (Pt) surfaces and nanoclusters has, in its preliminary stages, produced a highly accurate model of the relationship between volume and energy for platinum metal. Calculations have also determined the energy needed to form the Pt(111) surface, which is important in catalyzing many chemical reactions.

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 INCITE | 40 Million Core-Hours

## Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale

Electrochemical interfaces are responsible for the success of electrochemical energy conversion/storage systems, such as fuel cells and batteries, as well as the failure of materials caused by corrosion. This project aims to elucidate nanoscale and mesoscale mechanisms associated with electrochemical processes occurring at reactive material interfaces. Breakthroughs in the fundamental understanding of these interfaces are necessary in the design and development of novel oxide materials for energy applications.

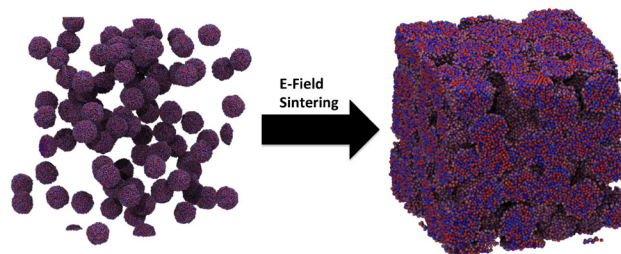
Dynamical electrochemical processes combine the remarkable complexity of many interfacial reactions, transport phenomena, and microstructural evolution with the formidable subtleties of material defect chemistry at the interface. Focusing on material synthesis and electrochemical interfaces, project researchers set out to understand these behaviors at the atomistic and molecular levels during an electric field-assisted oxide-sintering process.

Sintering—the process of welding together two metal powders at a diminished liquid phase—is well established, though the processes governing electric field sintering phenomena at the nanoscale were largely unexplored. Using representative oxide models of zirconia and ceria variants, researchers have shown that electric field-assisted sintering can be used to design oxide materials with modifications that would affect their functional properties.

Calculations of the atomistic scale and interfacial properties of nanoscale oxides and oxide heterostructures were conducted on Mira using the highly scalable molecular dynamics simulation code LAMMPS. ALCF computational scientists were instrumental in preparing this same code for a multimillion-cell reactive simulation of passive oxide growth, meant to accurately capture microstructural features and understand how to control oxygen stoichiometry in oxide thin films. Results have helped explain experimentally observed improvements in oxide quality resulting from the electric field-assisted sintering process.

Work on corrosion has, for the first time, elucidated the unique role of solvation dynamics in initiating corrosion at the nanoscale, and has shown that, at a critical threshold, concentrated chloride ions break up the ordered water layers and increase the rate of corrosion.

This research provides detailed insight into the critical early-stage formation of corrosion conditions on the nanosecond time scale and at the atomic level.



*Reactive molecular dynamics showing electric field sintering of FeOx nanoparticles to form a thin film.*

Image credit: Subramanian Sankaranarayanan, Argonne National Laboratory

### IMPACT

**A better understanding of reactive interfaces can enable the fabrication of novel architectures, materials, and structures that demonstrate unique functionalities and characteristics. The ability to computationally design advanced ceramic nanomaterials whose functional properties can be controlled with atomic precision is a critical starting point toward advancing energy technologies.**

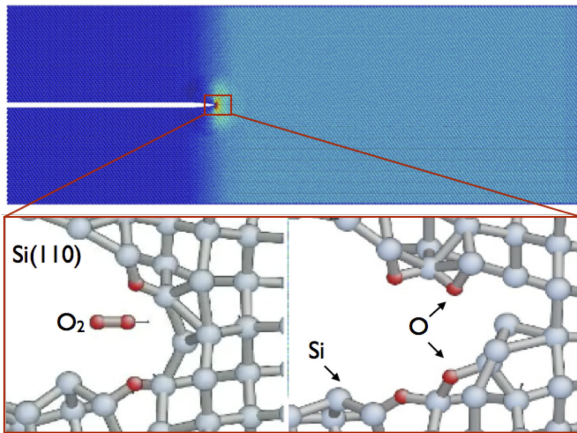


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INCITE | 125 Million Core-Hours



*Stress-corrosion cracking on the silicon (110) cleavage plane can be mediated by dissociative chemisorption of oxygen molecules. A large model system (top) is required to accurately model stress concentration, but QM accuracy is only needed in a small region near the crack tip (bottom).*

Image credit: James Kermode,  
King's College London

## SiO<sub>2</sub> Fracture: Chemo-mechanics with a Machine Learning Hybrid QM/MM Scheme

Understanding the chemo-mechanical phenomena that cause silicates to fracture would prove a great advantage to both enabling the process, as in large-scale mining, and eliminating it in products that rely on silicate materials. Researchers at King's College London are utilizing a hybrid multiscale computing tool on Mira to better understand stress corrosion/chemically activated crack propagation behaviors at both the macroscopic and microscopic levels.

An abundant component of Earth's geologic formations, silica is extracted during the preparation of mineral ores; and silicates are used widely in products as diverse as biomedical implants and semiconductors. A brittle material, silica is prone to stress-corrosion fractures which can lead to costly degradation and failures in these products. Until recently, their theoretical study had been difficult because of the high cost of experiments and tight chemo-mechanical coupling of chemistry and elastic fields, creating an inextricably multiscale problem.

The King's College research team applied a hybrid multiscale simulation program that combines various levels of theories to help describe the fracturing of silicon dioxide (SiO<sub>2</sub>). In this quantum mechanical/molecular mechanical (QM/MM) scheme, higher level theories account for the breaking of chemical bonds; the less expensive levels enable the inclusion of thermal fluctuations that link the microscopic behavior of these breaking bonds to the macroscopic stress that drives crack propagation.

As the INCITE project develops, the QM/MM approach will be coupled with a machine learning method, Learn on the Fly (LOTF), that allows for quantum mechanical accuracy on a large model system. In this approach, observed data is stored and used later to infer a solution to similar or recurring events, thus speeding the simulation.

The simulations have shown, thus far, that cracks in silicon can initiate and propagate in the presence of oxygen, even if the energy supplied by the load is insufficient to create new fracture surfaces in pure systems. These results were confirmed by experiments that showed no evidence of cracking in oxygen-free conditions. Access to Mira enabled a ten-fold increase in sampling time in these simulations. Further contributing to the project, ALCF staff helped port the researchers' code and improve the scalability of the LOTF method.

### IMPACT

**This research has implications for the manufacture of silica-based products resistant to fracture, and could significantly reduce energy and cost expenditures associated with mineral ore processing. The methodology used has potential future application in the study of a variety of materials.**

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ALCC | 250 Million Core-Hours

## Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions

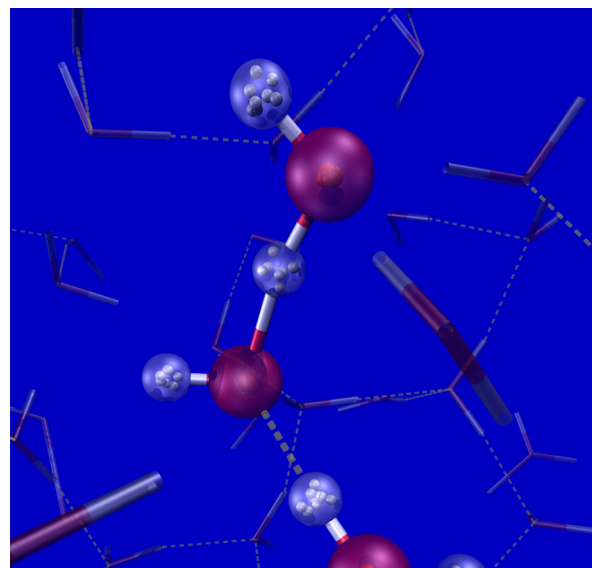
A highly accurate and detailed understanding of the microscopic structure of liquid water is critical to a number of fields, including energy storage, biochemistry, and the environmental sciences. For this ALCC project, researchers from Princeton University are using an innovative computational approach on Mira to study liquid water and aqueous ionic solutions at the atomic level with unprecedented accuracy.

At present, no experimental methodology exists to directly obtain the microscopic structure of liquid water. However, computer-based simulations can furnish such structural information. While *ab initio* molecular dynamics (AIMD) based on density functional theory is the most accurate and widely used computational methodology for modeling condensed phase systems, this approach has severe limitations when applied to liquid water.

To overcome these issues, the Princeton research team is combining novel algorithmic and theoretical developments to perform highly accurate benchmark atomistic simulations of liquid water on Mira. They are also applying this approach to aqueous ionic solutions that are relevant to the design of clean energy materials, such as electrolytes for aqueous-ion batteries.

The researchers have completed several production-level path integral (PI)-AIMD simulations of liquid water at the PBE, PBE+vdW, and PBE0+vdW levels of theory. These simulations allowed them to accurately capture the main experimental isotope effects in the oxygen-oxygen, oxygen-hydrogen, and hydrogen-hydrogen radial distribution functions of liquid water. The team also carried out large-scale PI-AIMD simulations to investigate the proton transfer mechanism in the fundamental hydronium ( $\text{H}_3\text{O}^+$ ) and hydroxide ( $\text{OH}^-$ ) ionic solutions (the models of acidic and basic conditions, respectively). The proton transfer rates from these simulations were found to be in excellent agreement with experimental data.

In addition, their work has determined the importance of exact exchange and non-local van der Waals (vdW) interactions in predicting the density ordering between crystalline ice and liquid water—an anomalous property of water that has posed a substantial challenge for this theory to date. The researchers have also investigated the importance of vdW/dispersion interactions in predicting the structure of weakly bound molecular crystals at finite temperatures and pressures.



Graphical snapshot of a proton transfer event taken from a PI-AIMD simulation of the solvated hydroxide ion. The atoms involved are represented by semi-transparent red (oxygen) and white (hydrogen) spheres.

Image credit: Roberto Car, Robert A. DiStasio Jr., Hsin-Yu Ko, and Biswajit Santra, Princeton University; Xifan Wu and Lixin Zheng, Temple University

### IMPACT

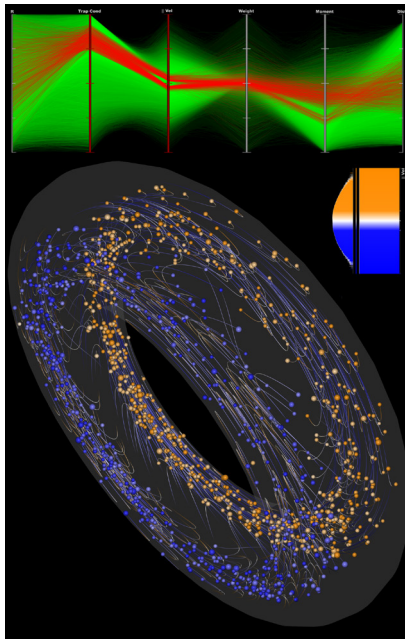
**These benchmark simulations are providing detailed knowledge of the microscopic structure of liquid water and aqueous ionic solutions with unprecedented accuracy. The results, which will be stored in a publicly available structural database, will serve as a valuable resource to inform further theoretical investigations and to help advance clean energy applications, such as the rational design of aqueous-ion batteries.**

**WILLIAM TANG**

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INCITE | 50 Million Core-Hours



*Particle visualization of a global gyrokinetic particle-in-cell simulation of microturbulence in a tokamak fusion device. This figure illustrates the dynamics of millions of particles moving primarily in the direction parallel to the magnetic field during the simulations. The class of particles highlighted are those in a magnetically trapped state with their parallel velocities close to zero.*

Image credit: Stephane Ethier, Princeton Plasma Physics Laboratory; Chad Jones and Kwan-Liu Ma, University of California, Davis

### IMPACT

**This work will provide valuable new insights on the long-standing challenge of how to reliably assess the influence of increased plasma size—especially at the largest scales—on the key confinement properties of fusion-grade magnetically confined plasmas.**

## Kinetic Simulations of Fusion Energy Dynamics at the Extreme Scale

With the potential to provide clean, safe, and abundant energy, nuclear fusion has been called the “holy grail” of energy production. This project will develop new capabilities to efficiently compute and determine how turbulent transport and associated confinement characteristics scale from present-generation laboratory plasmas to the much larger-scale burning plasmas in the cores of huge magnetic chambers, or tokamaks.

Studies on extreme-scale plasma turbulence have provided valuable new insights on the long-standing challenge of how the turbulent transport of plasma particles and their associated confinement scale from present-generation devices to much larger scales, such as that presented by the super tokamak ITER, currently under construction in Southern France.

Simulations of confinement physics for large-scale plasmas have been carried out for the first time with very high phase-space resolution and long temporal duration. These studies demonstrate that, as devices grow larger, improvement in confinement take place far more gradually and with significantly lower loss rates than less-powerful computer simulations have indicated in research carried out over the past decade.

The magnitude of turbulent losses in the Gyro-Bohm regime, where losses are independent of tokamak size, can be up to 50 percent lower than previously indicated. The actual transition from the Bohm regime, where turbulent losses increase with tokamak size, to the Gyro-Bohm regime follows a much more gradual trend.

Since the predictions from these more accurate simulations predict a lower overall loss rate of energy, this is actually a more favorable trend than previously predicted in lower resolution computations. With a clearer picture of the shape of this transition curve, scientists will be better able to understand and thereby influence the basic plasma physics involved in this phenomenon.

In order to achieve the physics fidelity and associated simulation resolution needed, researchers used the kinetic simulation capability of its primary project code, Gyrokinetic Toroidal Code-Princeton (GTC-P), running on Mira. A highly optimized particle-in-cell code, it is being used to study microturbulence in magnetically confined plasmas.

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 INCITE | 340 Million Core-Hours  
 ALCF 240 Million; OLCF 100 Million

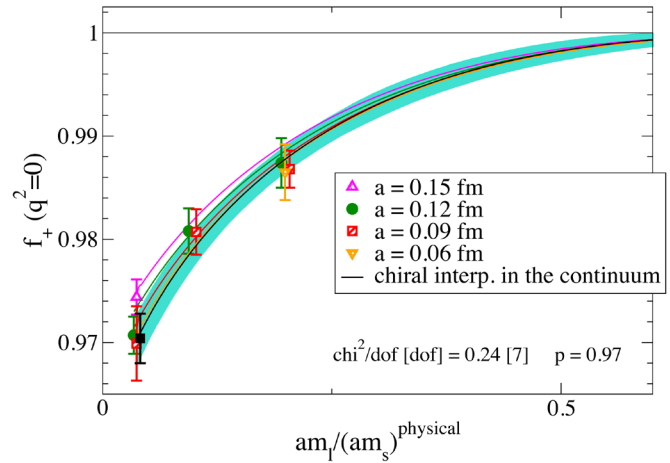
## Lattice QCD

One problem with the Standard Model of physics is the large number of unpredicted free parameters, like quark masses, the explanations for which still leave physicists stumped. This project endeavors to dramatically advance research in lattice quantum chromodynamics (QCD) and other strongly coupled field theories to search for evidence of a more fundamental theory that helps explain these mysteries.

One way of looking for evidence of new physics beyond the Standard Model is to use lattice QCD to calculate the model's processes very precisely, compare the results with experiments, and look for discrepancies. Utilizing INCITE computing resources, researchers from the USQCD Collaboration are generating fine-grained lattices with up, down, strange, and charm quarks at their physical mass values that enable full control of systematic errors for a number of key quantities, such as mass and decay constants.

As part of USQCD's work at the Intensity Frontier, the Domain-Wall Fermion and HISQ Fermion projects have begun generating ensembles of lattice configurations that may represent the most demanding lattice QCD simulations yet attempted. These calculations describe the light quarks, which are given their physical mass, and include the charm quark. This will allow, for the first time, calculations in which the intrinsic symmetry of the up and down quarks is faithfully reproduced. In addition, a wide variety of important quantities in QCD can be studied.

Expanding the Intensity Frontier research have been studies of highly improved staggered quarks (HISQ). Staggered quarks have proven to be particularly useful for making precise determinations of parameters of the Standard Model. The function for decay rate, or form factor, for the decay of a kaon into a pion and two leptons yields the most precise determination so far of the Cabibbo-Kobayashi-Maskawa (CKM) matrix element,  $|V_{us}|$ , the up-strange quark mixing parameter. When combined with the CKM matrix element  $|V_{ud}|$ , the up-down quark mixing parameter, obtained from nuclear beta decay, it shows a small, or two-sigma, discrepancy from the relation expected from the Standard Model. Discrepancies of that size are expected from time to time from statistical fluctuations, but an increase determined through improved theory or experiment could indicate new physics beyond the Standard Model.



The form factor for the decay of a kaon into a pion and two leptons. It yields the most precise determination so far of the CKM matrix element,  $|V_{us}|$ .

Image credit: A. Bazavov et al., Phys.Rev. Lett. 112 (2014) 112001; e-Print: arXiv:1312.1228

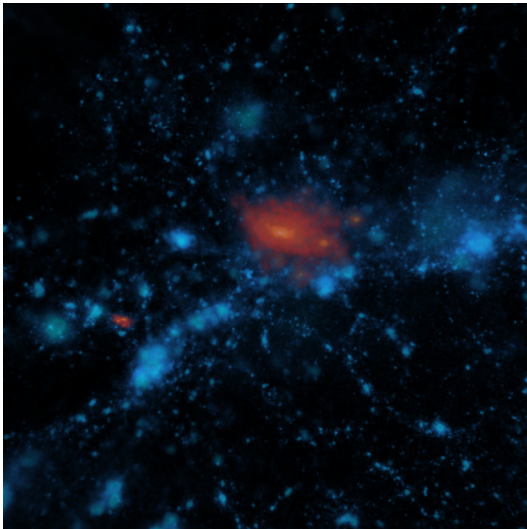
## IMPACT

The discovery of a true discrepancy between Standard Model predictions and experiment would lay the foundation for a new era in post-Standard Model particle physics.



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ALCC | 47 Million Core-Hours



Visualization of the dark matter distribution from one of the MockBOSS simulations. The simulation was carried out on 32,768 ranks on Mira covering a cosmological volume of 5,943 Mpc. The visualization shows a zoom-in to the output from only one rank, highlighting two massive dark matter clusters in red.

Image credit: Katrin Heitmann, Joseph Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory

## MockBOSS: Calibrating Boss Dark Energy Science with HACC

The cause of the universe's accelerated expansion is one of the great mysteries in physics today. Researchers are studying the phenomenon with cosmological surveys, such as the Baryon Oscillation Spectroscopic Survey (BOSS). To analyze and interpret survey results, a research team led by Argonne National Laboratory is using Mira to perform large-scale simulations of the universe to validate the observations and to serve as a defense mechanism against systematic uncertainties.

For this ALCC project, the researchers used ALCF computing resources to generate a set of very large volume simulations aimed at creating mock galaxy catalogs for BOSS. The simulations were performed with HACC (Hardware/Hybrid Accelerated Cosmology Code).

To analyze the BOSS data, a computationally feasible method was needed to generate covariance matrices and explore how the covariance matrices depend on the choice of the underlying cosmological input model. A brute-force approach would require thousands of large, high-resolution simulations, which was not possible with available computing resources.

To develop a more manageable approach, the researchers carried out a suite of test simulations that use a smaller number of time steps, reducing the computational time required by a factor of five. After receiving promising results from the test simulations, the team moved on to simulations that covered the full survey to explore six different cosmological models. For each model, they generated six simulations: one simulation at full-time resolution and five simulations with fewer time steps. These simulations were populated with galaxies to generate realistic galaxy catalogs that can be directly compared (in a statistical sense) with the observations. Researchers continue to analyze the simulation results.

### IMPACT

**This research will enhance interpretation of BOSS survey data, further our theoretical understanding of the universe's accelerated expansion, and deliver important insights for future surveys, such as the Large Synoptic Survey Telescope. The massive volume of the simulations will also enable researchers to look for rare events (e.g., determining the probability that a survey finds a massive cluster of galaxies in the early stage of the evolution of the universe).**

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ALCC | 19.5 Million Core-Hours

## Predictive Full-Scale Simulations of Fast Ignition of Fusion Targets

In the quest for fusion energy, it is imperative to understand the properties of laser-accelerated electrons in the context of fast ignition of inertial confinement fusion. Utilizing the largest 3D particle-in-cell (PIC) simulations to date, researchers are striving to understand how lasers transfer their energy to electrons, and how the properties of fast electrons depend on laser and fuel parameters.

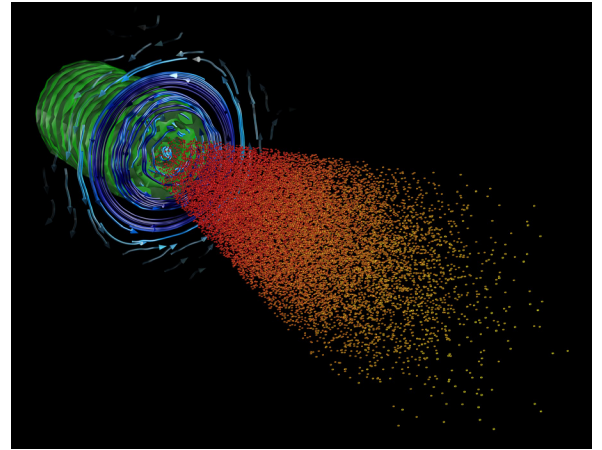
In the fast ignition route to fusion energy, a fusion fuel, or plasma, is heated and ignited by a single high-power laser that interacts with the surface of the compressed fuel and accelerates electrons. A large fraction of the laser's energy is transferred to the electrons, which then speed to the fuel's core and deposit this energy.

A team from Lawrence Livermore National Laboratory turned to Mira to perform 2D and 3D simulations of this fast ignition process at previously unattainable scales and resolution with the state-of-the-art PIC code OSIRIS.

In the largest 3D simulation of its kind, researchers modeled the interaction of the ignition laser with dense fuel plasma, accounting for different laser intensities, wavelength and spot sizes, and different plasma densities. Initial analysis indicates that the electron divergence is smaller than was initially assessed in earlier, smaller-scale simulations and, as a consequence, the energy deposition in the fuel is more efficient.

Researchers have also begun modeling the propagation of a fast electron beam on a dense plasma background to better understand the role of physical and numerical parameters on the energy exchange between beam and plasma. When resolution and particle interpolation order are carefully chosen, highly resolved simulations of typical, fast ignition conditions show that Ohmic heating—which occurs due to collision of the fast electrons with slower background plasma particles—dominates the energy losses when compared to collective plasma processes.

This finding suggests that the energy loss in the low-density region of the fuel is not significant and, therefore, a larger fraction of the energy is deposited in the center of the fuel, as required for efficient fusion energy production.



*Interaction of a fast-ignition-scale laser with a dense plasma. The laser field is shown in green, the blue arrows illustrate the magnetic field lines at the plasma interface, and the red/yellow spheres are the laser-accelerated electrons that will heat and ignite the fuel. Simulation performed with the particle-in-cell code OSIRIS on Sequoia at Lawrence Livermore National Laboratory.*

Image credit: Frederico Fiuza, Lawrence Livermore National Laboratory

## IMPACT

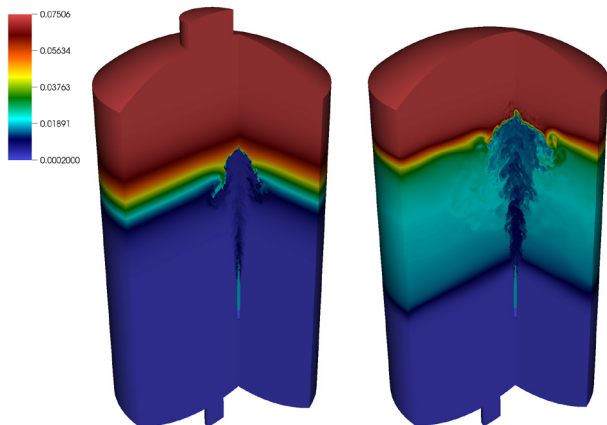
**Understanding the ignition laser/fuel interaction allows the ability to control the properties of fast electrons. This is critical to optimize the efficiency of fast ignition and make this approach viable to fusion energy. Moreover, the 3D simulation results are directly relevant to and important for their interpretation of today's experiments of intense laser-solid interactions.**

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INCITE | 60 Million Core-Hours



*This visualization depicts the helium mass fraction (red is high, dark blue is low) of the mixture of helium, oxygen, nitrogen, and water vapor inside the PANDA containment at early time (left) and late time with a simplified geometry (right). The containment vessel is 8 m x 4 m with an inlet pipe diameter of 7.5 cm.*

Image credit: Paul Fischer, Aleksander Obabko, and Ananias Tomboulides, Argonne National Laboratory

## Thermal Hydraulic Modeling: Cross-Verification, Validation, and Co-Design

Modeling and simulation tools are an intrinsic part of nuclear engineering research, but higher fidelity computational capabilities are needed to help advance nuclear energy technologies by resolving technical, cost, and safety issues. With this INCITE project, Argonne researchers seek to push the boundaries of thermal hydraulic modeling for design and validation efforts, including a benchmark study of results from PANDA, a large-scale thermal hydraulics test facility at the Paul Scherrer Institute in Switzerland.

When the Fukushima Daiichi nuclear meltdown occurred in 2011, the convection and mixing flow in the containment facility played an important role in the accident as buoyant hydrogen gas mixed with oxygen and detonated, resulting in significant destruction and radioactive pollution. Following the disaster, the Organization for Economic Cooperation and Development's Nuclear Energy Agency chose the PANDA experiment for a 2014 benchmark exercise to test the predictive capabilities of computational fluid dynamics (CFD) tools for the relevant flow physics. Specifically, the benchmark would test code predictions of multispecies convection in a notorious regime of transition from turbulent to laminar flow and from forced to natural convection. Accurate prediction of these phenomena is critical to understanding reactor behavior during accidents and will aid in the design of safer and more efficient nuclear reactors.

As part of this INCITE project, researchers are using the Argonne-developed Nek5000 code, an open-source CFD solver based on the spectral element method, to conduct a series of numerical experiments to optimize computational cost and accuracy in PANDA's flow regime. Designed to study buoyancy, convection, and mixing flows, the PANDA facility contains a well-defined gas mixture of helium and air at the top, and air below with measured stratification. A turbulent jet of air and buoyant helium injected into the vessel through the inlet pipe gradually erodes the initial stratification layer, posing significant challenges for accurate prediction of flow evolution.

With support from ALCF staff, the Argonne team made a number of insights while simulating this difficult flow regime with Nek5000, including the optimal meshing strategy and the best approach for modeling the inlet boundary. They developed and tested various approximations for modeling buoyancy and diffusion effects, and their impact on the flow solution accuracy and simulations costs. The results will be compared with experimental benchmark data to validate Nek5000 in this flow regime and with fast lower fidelity methods to improve their accuracy.

### IMPACT

**This project is simulating the complex turbulent flows in the benchmark regime studied at the PANDA experiment in Switzerland, providing important insights for flow physics modeling and associated computational cost and accuracy trade-offs. The results, which are important for prediction of nuclear reactor containment accident scenarios, will aid in the design of safer and more efficient nuclear reactors.**

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ALCC | 12.5 Million Core-Hours

ALCF 7.5 Million; OLCF 5 Million

## Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime

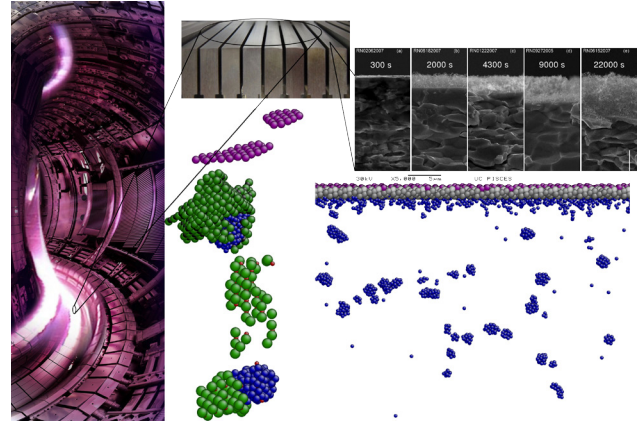
Providing energy from terrestrial nuclear fusion reactions is among the great scientific and engineering challenges of our time. One possible route to fusion energy is magnetically confined plasma reactors. This project will study the reaction of helium plasma on specific surface structures of tungsten, the proposed material for large tokamak divertors, which are responsible for the removal of fusion reaction by-products.

Tungsten is currently the material of choice for the divertors in prototype magnetic-confinement nuclear fusion reactors, such as the super tokamak ITER, due to its high thermal conductivity and related high-temperature properties.

Research efforts have focused on large-scale molecular dynamics (MD) simulations to develop an atomistic database on the helium bubble formations in tungsten. ALCF was integral in helping researchers skillfully run the MD code LAMMPS on Mira, providing a detailed microscopic picture of helium plasma structures on the surface of tungsten.

Simulation results have focused on implanting helium gas atoms below low index (100), (110), or (111) tungsten surfaces. The most current and significant scientific results are associated with how the trap mutation processes – in which a pressurized helium atom cluster ‘knocks’ a tungsten lattice site to create a tungsten vacancy – are modified in the presence of a free surface. There is marked difference in the helium retained between (001) or (011) and the (111) or (211) surfaces. This suggests that a mechanism exists that prevents helium from leaving the surface in the (111) or (211) cases that does not exist for the other surface orientations, and that this mechanism is quite strong.

Where (001) or (011) surfaces require a cluster of helium atoms before the gas pressure is sufficient to create adatoms and other surface damage, MD simulations have shown that this process can occur at the size of just a single helium atom, when helium is below a (111) surface. This results in a very large concentration of helium atoms in substitutional tungsten positions just a few monolayers below the surface. The presence of this helium layer may substantially influence the sputtering and erosion behavior of tungsten.



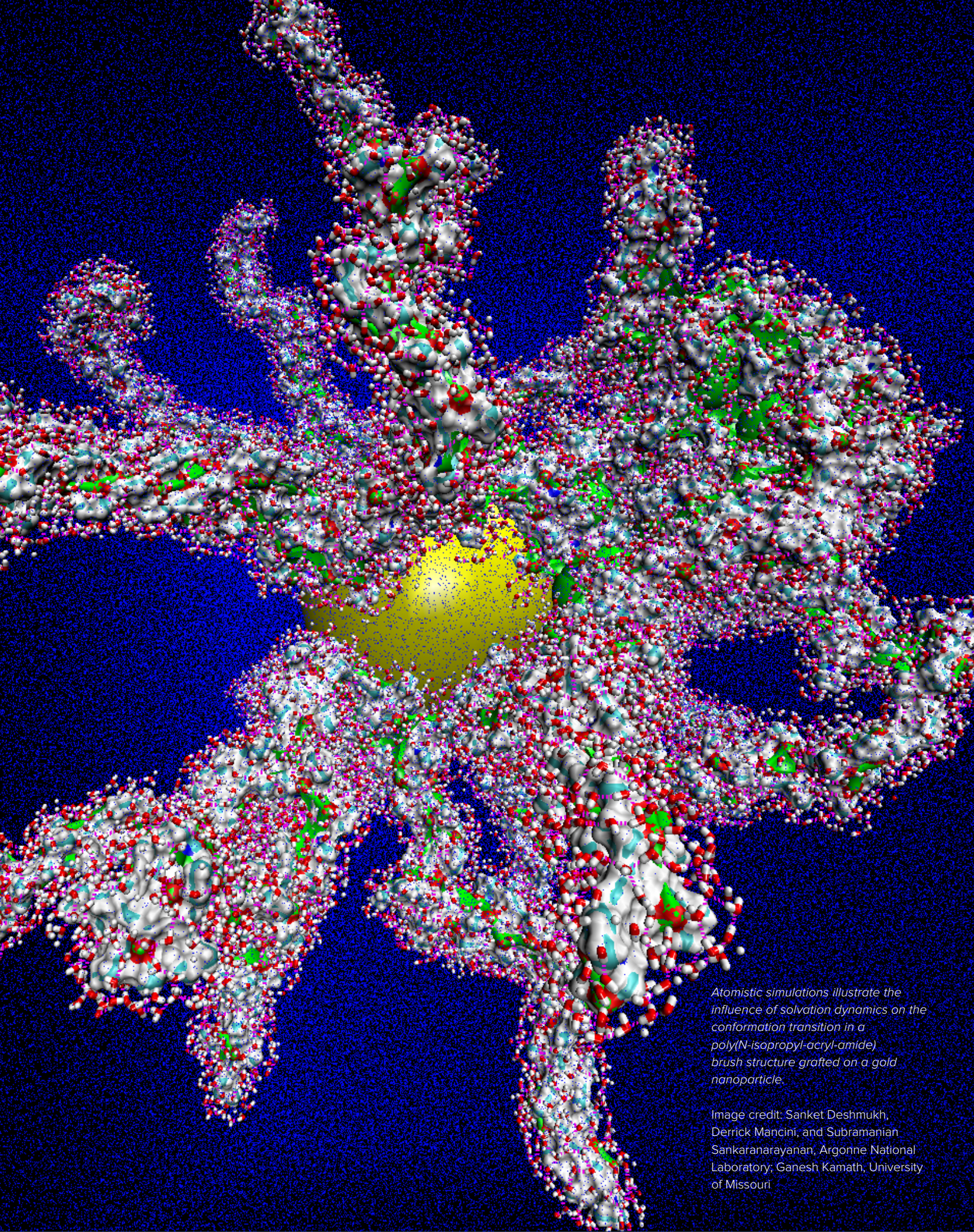
The divertor in a fusion tokamak must withstand severe plasma surface interactions. Top right inset shows tungsten surface morphology following helium plasma exposure. Molecular dynamics simulations have identified growing helium bubbles (blue spheres) that produce surface roughness responsible for nanoscale fuzz.

Image credit: Brian D. Wirth, University of Tennessee, Knoxville

### IMPACT

The results of this work may indicate that some surface orientations are preferable to others for the exposed surfaces of plasma-facing components and, thus, provide a greater physical understanding and predictive modeling capability for materials design of the ITER divertor.



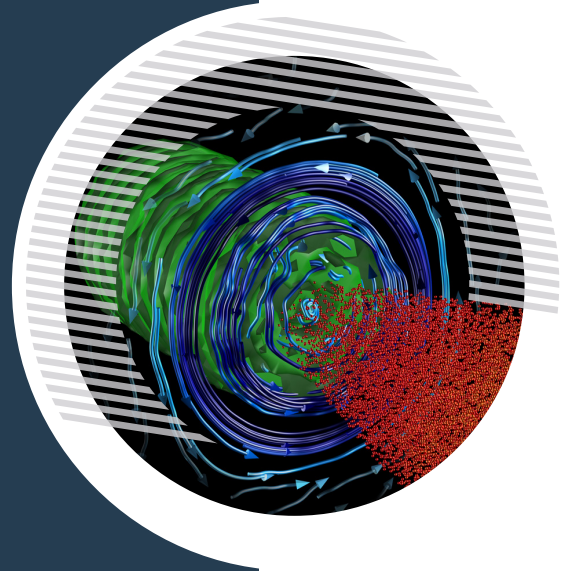


*Atomistic simulations illustrate the influence of solvation dynamics on the conformation transition in a poly(N-isopropyl-acryl-amide) brush structure grafted on a gold nanoparticle.*

Image credit: Sanket Deshmukh, Derrick Mancini, and Subramanian Sankaranarayanan, Argonne National Laboratory; Ganesh Kamath, University of Missouri



# EXPERTISE AND RESOURCES



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## The **ALCF** has assembled a **world-class team** of experts to help maximize the use of ALCF computing systems.

**Catalysts** are computational scientists who work directly with project teams to maximize and accelerate their research efforts. This includes helping users to port, scale, tune, and improve codes and algorithms. The catalyst team has domain expertise in areas such as chemistry, materials science, fusion, nuclear physics, plasma physics, computer science, engineering, and Earth science.

**Performance Engineers** help users achieve optimal performance on ALCF resources by working with them to port, tune, and parallelize scientific applications and other software. This includes assessing and improving the algorithms used by applications and the techniques used to implement those algorithms.

**Data Analytics and Visualization Experts** facilitate the use of tools and methods for high-performance post processing of large datasets, interactive data exploration, batch visualization, and production visualization.

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

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

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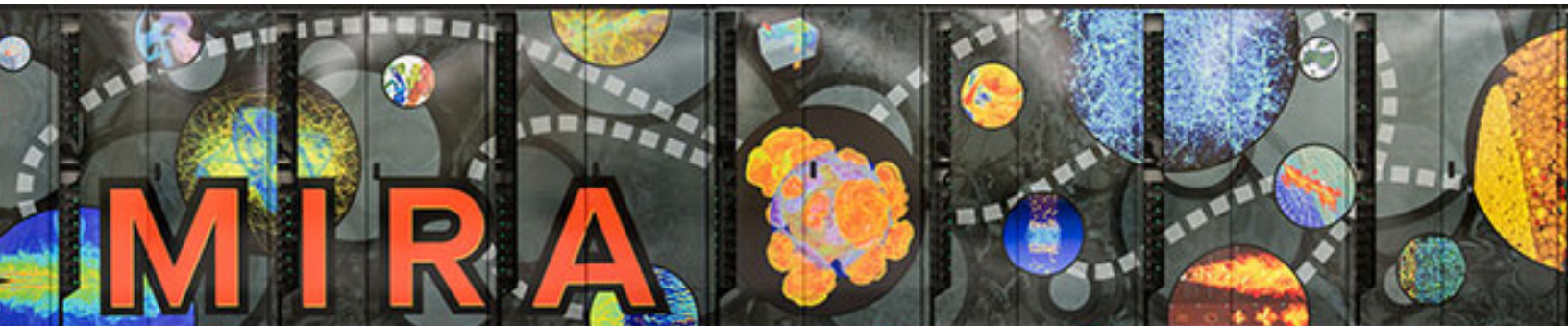
# COMPUTING RESOURCES

## Mira

Mira, the ALCF's 10-petaflops supercomputer, opens the door for scientists to analyze data more efficiently, design products more quickly, and address some of society's biggest problems in ways that would otherwise be impossible. An engineering marvel, the system is capable of carrying out 10 quadrillion calculations per second.

Mira is also among the most energy-efficient supercomputers, saving considerable energy through innovative chip designs and a unique water-cooling system.

- 48 racks
- Sixteen 1600 MHz PowerPC A2 cores per node
- 49,152 nodes
- 786,432 cores
- 768 TiB RAM
- 5D torus interconnect
- 384 I/O nodes
- Peak performance of 10 petaflops





## Cetus

The primary role of Cetus is to run small jobs to debug problems that occurred on Mira. Cetus shares the same software environment and file systems as Mira.

- 4 racks
- 4,096 nodes
- 64 TiB RAM
- 5D torus interconnect
- 32 I/O nodes
- Peak performance of 838 teraflops

## Vesta

Vesta is the ALCF's test and development platform, serving as a launching pad for researchers preparing to use Mira. Vesta has the same architecture as Mira, but on a much smaller scale.

- 2 racks
- 2,048 nodes
- 32 TiB RAM
- 5D torus interconnect
- 32 I/O nodes
- Peak performance of 419 teraflops

## Tukey

Tukey is the ALCF's analysis and visualization cluster. Equipped with state-of-the-art graphics processing units (GPUs), Tukey converts computational data from Mira into high-resolution visual representations. The resulting images, videos, and animations help users to better analyze and understand the data generated by Mira. Tukey can also be used for statistical analysis, helping to pinpoint trends in the simulation data.

Additionally, the system is capable of preprocessing efforts, such as meshing, to assist users preparing for Mira simulations. Tukey shares the Mira network and parallel file system, enabling direct access to Mira-generated results.

Each Tukey node has:

- Two 2 GHz 8-core AMD Opteron CPUs
- 2 NVIDIA Tesla M2070 GPUs
- 64 GB of Ram

The full Tukey system has:

- 96 nodes
- 1,536 cores
- QDR InfiniBand interconnect
- 6 TiB of RAM
- 11 TiB of GPU RAM
- GPU peak performance (aggregate) of over 99 teraflops (double precision)

## 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 GPFS file system to access the storage.

**Tape Storage:** The ALCF's Blue Gene/Q supercomputer has two 10,000-slot libraries using LTO 4 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 16-24 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.

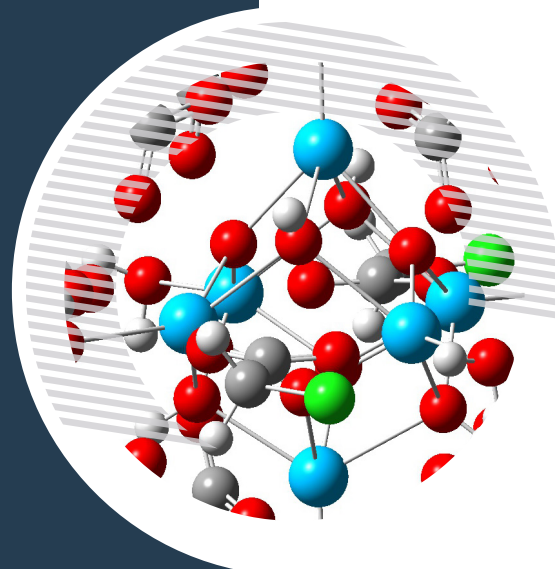
The ALCF connects to other research institutions using a total of 100 Gb/s of public network connectivity. Scientists can transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and Internet2.



*Visualization of the dark matter distribution from one of the MockBOSS simulations. The simulation was carried out on 32,768 ranks on Mira covering a cosmological volume of 5,943 Mpc. The visualization shows a zoom-in to the output from only one rank, highlighting two massive dark matter clusters in red.*

Image credit: Katrin Heitmann, Joseph Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory

# 2014 ALCF PROJECTS



## 2014 INCITE PROJECTS

**Biological Sciences****Multiscale Simulations of Human Pathologies**

George Karniadakis, Brown University

Allocation: 45 Million Core-Hours

**Studies of Large Conformational Changes in Biomolecular Machines**

Benoît Roux, University of Chicago

Allocation: 55 Million Core-Hours

**Chemistry****Computational Actinide Chemistry: Reliable Predictions and New Concepts**

David Dixon, University of Alabama

Allocation: 250 Million Core-Hours

ALCF: 100 Million; OLCF: 150 Million

**DNS of Forced- and Auto-Ignition in Spherical and Engine-Like Geometries**

Christos Frouzakis, Swiss Federal Institute of Technology Zurich

Allocation: 100 Million Core-Hours

**First-Principles Simulations of High-Speed Combustion and Detonation**

Alexei Khokhlov, University of Chicago

Allocation: 150 Million Core-Hours

**Solving Petascale Public Health and Safety Problems Using Uintah**

Martin Berzins, University of Utah

Allocation: 200 Million Core-Hours

**Upscaling Laws in Premixed Explosions**

Thierry Poinsot, CERFACS

Allocation: 86 Million Core-Hours

**Vibrational and Optical Spectroscopy of Electrolyte/Solid Interfaces**

Giulia Galli, University of Chicago;

Francois Gygi, University of California, Davis

Allocation: 70 Million Core-Hours

**Computer Science****Dynamic and Adaptive Parallel Programming for Exascale Research**

Robert Harrison, Brookhaven National Laboratory

Allocation: 20 Million Core-Hours

**Performance Evaluation and Analysis Consortium (PEAC) End Station**

Leonid Oliker, Lawrence Berkeley National Laboratory

Allocation: 75 Million Core-Hours

ALCF: 30 Million; OLCF: 45 Million

**Scalable System Software for Parallel Programming**

Robert Latham, Argonne National Laboratory

Allocation: 25 Million Core-Hours

**Earth Science****CESM Century-Scale Climate Experiments with a High-Resolution Atmosphere**

Warren Washington, University Corporation for Atmospheric Research

Allocation: 102.8 Million Core-Hours

**Chombo-Crunch: Modeling Pore-Scale Reactive Transport in Carbon Sequestration**

David Trebotich, Lawrence Berkeley National Laboratory

Allocation: 80 Million Core-Hours

**High-Frequency Physics-Based Earthquake System Simulations**

Thomas Jordan, University of Southern California

Allocation: 112.2 Million Core-Hours

ALCF: 64.2 Million; OLCF: 48 Million

**High-Resolution Simulation for Climate Means, Variability, and Extreme**

Mark Taylor, Sandia National Laboratories

Allocation: 150 Million Core-Hours

ALCF: 50 Million; OLCF: 100 Million



## Engineering

### **Adaptive Detached Eddy Simulation of a High Lift Wing with Active Flow Control**

Kenneth Jansen, University of Colorado

Allocation: 66 Million Core-Hours

### **Combustion Stability in Complex Engineering Flows**

Lee Shunn, Cascade Technologies

Allocation: 100 Million Core-Hours

### **Large Eddy Simulations of Combustor Liner Flows**

Anne Dord, GE Global Research

Allocation: 75 Million Core-Hours

### **Parameter Studies of Boussinesq Flows**

Susan Kurien, Los Alamos National Laboratory

Allocation: 50 Million Core-Hours

## Materials Science

### **Computational Design of Novel Multiscale Concrete Rheometers**

William George, National Institute of Standards and Technology

Allocation: 40 Million Core-Hours

### **Correlated Electrons in Photoactive and Superconducting Materials**

Lucas Wagner, University of Illinois at Urbana-Champaign

Allocation: 60 Million Core-Hours

### **Molecular Engineering through Free Energy Mapping**

Juan de Pablo, University of Chicago

Allocation: 60 Million Core-Hours

### **Non-Covalent Bonding in Complex Molecular Systems with Quantum Monte Carlo**

Dario Alfé, University College London

Allocation: 126 Million Core-Hours

ALCF: 56 Million; OLCF: 70 Million

### **Petascale Simulations of Self-Healing Nanomaterials**

Rajiv Kalia, University of Southern California

Allocation: 200 Million Core-Hours

### **Predictive Materials Modeling for Li-Air Battery Systems**

Larry Curtiss, Argonne National Laboratory

Allocation: 100 Million Core-Hours

### **QMC Simulations Database for Predictive Modeling and Theory**

David Ceperley, University of Illinois at Urbana-Champaign

Allocation: 200 Million Core-Hours

ALCF: 100 Million; OLCF: 100 Million

### **Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale**

Subramanian Sankaranarayanan, Argonne National Laboratory

Allocation: 40 Million Core-Hours

### **SiO<sub>2</sub> Fracture: Chemo-mechanics with a Machine Learning Hybrid QM/MM Scheme**

James Kermode, King's College London

Allocation: 125 Million Core-Hours

### **Turbulent Rayleigh-Bénard Convection at High Rayleigh and Low Prandtl Numbers**

Janet Scheel, Occidental College

Allocation: 40 Million Core-Hours

## Physics

### **Cosmological Simulations for Large-Scale Sky Surveys**

Salman Habib, Argonne National Laboratory

Allocation: 200 Million Core-Hours

ALCF: 100 Million; OLCF: 100 Million

### **High-Fidelity Simulation of Tokamak Edge Plasma Transport**

Choong-Seock Chang, Princeton Plasma Physics Laboratory

Allocation: 229 Million Core-Hours

ALCF: 100 Million; OLCF: 129 Million

**Intensity-Dependent Dynamics in  
Fermilab and CERN Accelerators**

James Amundson, Fermilab  
Allocation: 50 Million Core-Hours

**Kinetic Simulations of Fusion Energy  
Dynamics at the Extreme Scale**

William Tang, Princeton University  
Allocation: 50 Million Core-Hours

**Lattice QCD**

Paul Mackenzie, Fermilab  
Allocation: 340 Million Core-Hours  
ALCF: 240 Million; OLCF: 100 Million

**Nuclear Structure and Nuclear Reactions**

James Vary, Iowa State University  
Allocation: 204 Million Core-Hours  
ALCF: 100 Million; OLCF: 104 Million

**Particle Acceleration in Shocks: From  
Astrophysics to Laboratory In Silico**

Frederico Fiuza, Lawrence Livermore National  
Laboratory  
Allocation: 120 Million Core-Hours

**Petascale Simulations of Inhomogeneous  
Alfvén Turbulence in the Solar Wind**

Jean C. Perez, University of New Hampshire  
Allocation: 100 Million Core-Hours

**Simulation of Laser-Plasma Interaction in  
National Ignition Facility Experiments**

Steven Langer, Lawrence Livermore National  
Laboratory  
Allocation: 200 Million Core-Hours

**Thermal Hydraulic Modeling: Cross-  
Verification, Validation, and Co-Design**

Paul Fischer, Argonne National Laboratory  
Allocation: 60 Million Core-Hours

**Thermodynamics of Quark Flavors  
from Lattice QCD**

Rene Bellwied, University of Houston  
Allocation: 120 Million Core-Hours

## 2013-2014 ALCC PROJECTS

### Biological Sciences

**Protein Binding and Interaction Analysis of  
Human Pathogen Protein Targets**

T. Andrew Binkowski, Argonne National  
Laboratory  
Allocation: 22.8 Million Core-Hours

### Earth Science

**Chombo-Crunch: Advanced Simulation of  
Subsurface Flow and Reactive Transport  
Processes Associated with Carbon  
Sequestration**

David Trebotich, Lawrence Berkeley  
National Laboratory  
Allocation: 100 Million Core-Hours  
ALCF: 80 Million; NERSC: 20 Million

**Multiscale Modeling of Dynamic Arctic  
Landscapes in a Changing Climate**

Richard Mills, Oak Ridge National Laboratory  
Allocation: 30 Million Core-Hours

### Engineering

**Does a Turbulent Duct Flow Ever Become  
Two-Dimensional?**

Hassan Nagib, Illinois Institute of Technology/  
KTH Mechanics, Sweden  
Allocation: 11 Million Core-Hours

**Petascale Thermal Hydraulic Simulations in  
Support of CESAR**

Elia Merzari, Argonne National Laboratory  
Allocation: 80 Million Core-Hours

**U.S. Russia Collaboration on Cross-Verification  
and Validation in Thermal Hydraulics:**

**Nek5000, Cfoam-CABARET, and Conv3D,  
Simulations of MATiS and MAX Experiments**  
Aleksandr Obabko, Argonne National Laboratory  
Allocation: 44 Million Core-Hours

**Wall Modeling and Primary Atomization for Predictive Large Eddy Simulation of Airframes, Jet Engines and Jet Noise**

Parviz Moin, Stanford University  
Allocation: 150 Million Core-Hours

## Materials Science

**Atomistic Simulations of Nanoscale Oxides and Oxide Interfaces**

Subramanian Sankaranarayanan, Argonne National Laboratory  
Allocation: 120 Million Core-Hours

**Dynamics of Conformational Transition in Polymer-Grafted Nanoparticles**

Subramanian Sankaranarayanan, Argonne National Laboratory  
Allocation: 170 Million Core-Hours

**First-Principles Investigations of Adsorbate-Metal Interactions: Quantum Monte Carlo and Ab Initio Molecular Dynamics Simulations**

Jeffrey Greeley, Purdue University  
Allocation: 75 Million Core-Hours  
ALCF: 50 Million; OLCF: 25 Million

**First-Principles Investigation of Oxygen Defects in Metal/Oxide/Metal Heterostructures: Structure, Energetics, and Transport in the Quantum Regime**

Olle Heinonen, Argonne National Laboratory  
Allocation: 50 Million Core-Hours

**Large-Scale Computation for Discovery and Design of Excited-State Phenomena in Next-Generation Energy Conversion Materials**

Jeffrey B. Neaton, Lawrence Berkeley National Laboratory  
Allocation: 41 Million Core-Hours  
ALCF: 23 Million; NERSC: 18 Million

## Physics

**Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions**

Robert A. DiStasio Jr., Princeton University  
Allocation: 250 Million Core-Hours

**Large Eddy Simulation of SFR Assembly Inlets**

Paul Fischer, Argonne National Laboratory;  
James Tallman, General Electric  
Allocation: 60 Million Core-Hours

**MockBOSS: Calibrating Boss Dark Energy Science with HACC**

Katrin Heitmann, Argonne National Laboratory  
Allocation: 47 Million Core-Hours

**Petascale Simulation of Laser Plasma Interactions Relevant to Inertial Fusion Energy**

F.S. Tsung, University of California, Los Angeles  
Allocation: 40 Million Core-Hours

**Predictive Full-Scale Simulations of Fast Ignition of Fusion Targets**

Frederico Fiuza, Lawrence Livermore National Laboratory  
Allocation: 19.5 Million Core-Hours

**Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime**

Brian Wirth, Oak Ridge National Laboratory  
Allocation: 12.5 Million Core-Hours  
ALCF: 7.5 Million; OLCF: 5 Million

## 2014-2015 ALCC PROJECTS

### Biological Sciences

**Applying Breakthroughs in Protein Structure Calculation to the Creation of Designer Enzymes**

David Baker, University of Washington  
Allocation: 200 Million Core-Hours

### Chemistry

**Influence of Morphology on Proton Transport in Proton Exchange Membrane**

Gregory Voth, University of Chicago/Argonne National Laboratory  
Allocation: 57.6 Million Core-Hours

**Large-Scale Turbulent Clean Coal Combustion**

Martin Berzins, University of Utah  
 Allocation: 40 Million Core-Hours  
 ALCF: 10 Million; OLCF: 30 Million

**Computer Science****Hobbes: Operating System and Runtime Research for Extreme Scale**

Ron Brightwell, Sandia National Laboratories  
 Allocation: 40 Million Core-Hours  
 ALCF: 5 Million; NERSC: 5 Million; OLCF: 30 Million

**Earth Science****Delivering the Department of Energy's Next-Generation High-Resolution Earth System Model**

Peter Thornton, Oak Ridge National Laboratory  
 Allocation: 137 Million Core-Hours  
 ALCF: 107 Million; OLCF: 30 Million

**Engineering****Amplitude Modulation of Wind Turbine Noise**

Sanjiva Lele, Stanford University  
 Allocation: 36.5 Million Core-Hours

**Petascale Simulations in Support of CESAR**

Elia Merzari, Argonne National Laboratory  
 Allocation: 80 Million Core-Hours

**Predictive Large Eddy Simulation of Jet Fuel Atomization, High Lift Airframes, and Reacting Supersonic Turbulent Flows on Unstructured Grids**

Parviz Moin, Stanford University  
 Allocation: 120 Million Core-Hours

**Understanding Secondary Motions and Their Impact in Modeling Turbulent Flows**

Hassan Nagib, Illinois Institute of Technology  
 Allocation: 11 Million Core-Hours

**Materials Science****Interfaces in Organic and Hybrid Photovoltaics**

Noa Marom, Tulane University  
 Allocation: 105 Million Core-Hours  
 ALCF: 75 Million; NERSC: 30 Million

**Nanostructure-Enhanced Chemical Reactivity and Detonation in Energetic Materials**

Aidan Thompson, Sandia National Laboratories  
 Allocation: 80 Million Core-Hours

**Prediction and Design of Energy Materials by Petascale Evolutionary Algorithm Simulations**

Giancarlo Trimarchi, Northwestern University  
 Allocation: 30 Million Core-Hours

**Physics****Composite Higgs Theory Beyond the Standard Model and the 14 TeV Upgrade of the Large Hadron Collider**

Julius Kuti, University of California, San Diego  
 Allocation: 88.7 Million Core-Hours

**Cosmic Frontier Computational End-Station**

Salman Habib, Argonne National Laboratory  
 Allocation: 176 Million Core-Hours  
 ALCF: 100 Million; NERSC: 76 Million

**Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An Ab Initio Study of Liquid Water**

Robert A. DiStasio Jr., Princeton University  
 Allocation: 350 Million Core-Hours

**Simulation of Large Hadron Collider Events Using Leadership Computing**

Thomas LeCompte, Argonne National Laboratory  
 Allocation: 52 Million Core-Hours  
 ALCF: 50 Million; NERSC: 2 Million

**Turbulent Multiphase Flows for Nuclear Reactor Safety**

Igor A. Bolotnov, North Carolina State University  
 Allocation: 76.8 Million Core-Hours



**Understanding Helium Plasma Mediated Tungsten Surface Response to Better Predict Fusion Plasma Facing Component Performance in ITER**

Brian Wirth, University of Tennessee  
Allocation: 96 Million Core-Hours  
ALCF: 66 Million; OLCF: 30 Million

**Validation Studies of Gyrokinetic Simulations to Understand the Coupling of Ion and Electron Scale Turbulence in Tokamak Plasmas**

Christopher Holland, University of California, San Diego  
Allocation: 140 Million Core-Hours  
ALCF: 90 Million; NERSC: 50 Million

## 2014 DIRECTOR'S DISCRETIONARY PROJECTS

The following list provides a sampling of the many DD projects at the ALCF.

### Biological Sciences

**A Microscopic Perspective on Outer Membrane Remodeling and Antimicrobial Peptide Resistance**

Roberto D. Lins, Universidade Federal de Pernambuco  
Allocation: 3 Million Core-Hours

**Ab Initio Level Calculations of Infrared and Raman Spectra of Biomolecules**

Shinichiro Nakamura, RIKEN  
Allocation: 5 Million Core-Hours

**ATP Transport in VDAC**

Sergei Noskov, University of Calgary  
Allocation: 2 Million Core-Hours

**Characterizing Large-Scale Structural Transitions in Membrane Transporters**

Emad Tajkhorshid, University of Illinois at Urbana-Champaign  
Allocation: 1 Million Core-Hours

**Computing 3D Structures of Large RNA from Small-Angle X-ray Scattering Data and Secondary Structure**

Yuba Bhandari and Yun-Xing Wang, National Cancer Institute  
Allocation: 4 Million Core-Hours

**Rational Design of Selective ALK2 Inhibitors**

Yun Luo, Western University of Health Sciences  
Allocation: 8 Million Core-Hours

**Towards Breakthroughs in Protein Structure Calculation and Design**

David Baker, University of Washington  
Allocation: 20 Million Core-Hours

### Chemistry

**Computational Studies of the Topological Properties of Micellar Solutions**

Subas Dhakal, Syracuse University  
Allocation: 3 Million Core-Hours

**Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow**

Christos Frouzakis, Swiss Federal Institute of Technology Zurich  
Allocation: 10 Million Core-Hours

**High Accuracy Predictions of the Bulk Properties of Water**

Graham Fletcher, Argonne National Laboratory  
Allocation: 3 Million Core-Hours

**Investigation of Catalytic Properties of Nanoclusters**

Leonardo Spanu, Shell International E&P, Inc.  
Allocation: 2 Million Core-Hours

**Massively Parallel Quantum Dynamics**

Bill Poirier, Texas Tech University  
Allocation: 14 Million Core-Hours

**Multistate Reactive Molecular Dynamics:  
Development of Electrochemical and  
Fragment Molecular Orbital Methods**

Gregory A. Voth, University of Chicago/Argonne  
National Laboratory  
Allocation: 2 Million Core-Hours

**Potential Energy Surfaces for Simulating  
Complex Chemical Processes**

Donald Truhlar, University of Minnesota  
Allocation: 4.9 Million Core-Hours

## Computer Science

### ICEE

John Wu, Lawrence Berkeley National  
Laboratory  
Allocation: 1.5 Million Core-Hours

**Scalable Data Management Analysis and  
Visualization**

Michael E. Papka, Argonne National Laboratory  
Allocation: 2.5 Million Core-Hours

**Scaling the Toolkit for Extreme Climate  
Analysis on Blue Gene/Q Systems**

Venkatram Vishwanath, Argonne National  
Laboratory  
Allocation: 4 Million Core-Hours

## Earth Science

**Development of Fire Map 1: Fire Threat  
to Utilities**

Timothy Brown, Desert Research Institute  
Allocation: 8 Million Core-Hours

**Evaluation of Mesoscale Atmospheric  
Model for Contrail Cirrus**

Roberto Paoli, CERFACS  
Allocation: 9 Million Core-Hours

## Engineering

**Direct Numerical Simulations of High Reynolds  
Number Turbulent Channel Flow**

Robert Moser, University of Texas at Austin  
Allocation: 1 Million Core-Hours

**Development of Predictive Multidimensional  
Combustion Modeling Capability with Detailed  
Chemistry**

Sibendu Som, Argonne National Laboratory  
Allocation: 1.5 Million Core-Hours

**Scalable Implementation of Weighted,  
Non-Linear Compact Scheme**

Debojyoti Ghosh, Argonne National Laboratory  
Allocation: 2 Million Core-Hours

**Simulation of a Shock-Boundary-Layer  
Interaction**

Philippe Spalart, Boeing Commercial Airplanes  
Allocation: 2 Million Core-Hours

**Simulations of the Effects of Vacancies on the  
Absorption Spectrum of h-BN**

Lucy Shi, University of Illinois at Chicago  
Allocation: 5 Million Core-Hours

**Studying Turbulence Using Numerical  
Simulation**

Curtis Hamman, Stanford University  
Allocation: 5 Million Core-Hours

**TACOMA Porting and Scaling Study**

Brian E. Mitchell, GE Global Research  
Allocation: 2 Million Core-Hours

## Materials Science

**Computations for the Development of the  
Nanoporous Materials Genome**

J. Ilja Siepmann, University of Minnesota  
Allocation: 8.1 Million Core-Hours

**h-BN-Water Interaction using Quantum Monte  
Carlo Calculation**

N. R. Aluru, University of Illinois at Urbana-  
Champaign  
Allocation: 1 Million Core-Hours

**Multiscale Modeling of Materials Under  
Extreme Dynamic Environments Through  
Large-Scale Computer Simulations**

Mauricio Ponga, California Institute of  
Technology  
Allocation: 6.1 Million Core-Hours

### **Nanostructure-Enhanced Detonation in Energetic Materials**

Tzu-Ray Shan, Sandia National Laboratories  
Allocation: 7.5 Million Core-Hours

### **Toward Crystal Engineering from First Principles**

Noa Marom, University of Texas at Austin  
Allocation: 2 Million Core-Hours

### **Understanding the Mechanism of Ion Stripping and Depositions at the Anode Materials in Novel Multivalent Ion Batteries**

Gerbrand Ceder, Massachusetts Institute of Technology  
Allocation: 1 Million Core-Hours

## **Mathematics**

### **Optimization of Stochastic Power Grid Systems**

Cosmin Petra, Argonne National Laboratory  
Allocation: 2.5 Million Core-Hours

## **Physics**

### **Calculation of Nuclear Matrix Element of Neutrinoless Double-Beta Decay**

Jun Terasaki, University of Tsukuba  
Allocation: 6.6 Million Core-Hours

### **Cosmic Reionization on Computers**

Nickolay Y. Gnedin, Fermilab/University of Chicago  
Allocation: 3.5 Million Core-Hours

### **Grid-Enabling High-Performance Computing for ATLAS**

Thomas J. LeCompte, Argonne National Laboratory  
Allocation: 3.1 Million Core-Hours

## ALCF.ANL.GOV

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

The ALCF is supported by DOE’s Office of Science, Advanced Scientific Computing Research (ASCR) program.

### **About Argonne National Laboratory**

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

## AVAILABILITY OF THIS REPORT (ANL/ALCF-14/2)

Online Access: U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via DOE’s SciTech Connect (<http://www.osti.gov/scitech/>)

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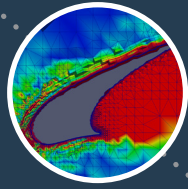
U.S. Department of Energy  
Office of Scientific and Technical Information  
P.O. Box 62  
Oak Ridge, TN 37831-0062  
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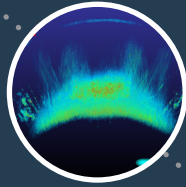
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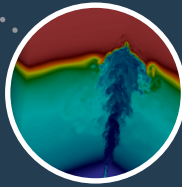
## FEATURED IMAGES



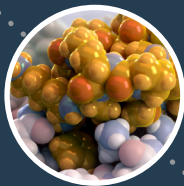
*Illustration of mesh adaptation with a slice through the mesh of a three element high lift wing (slat and main wing view).*  
Image credit: Kenneth Jansen, University of Colorado



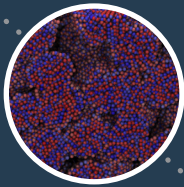
*A volume visualization of the laser light that has been backscattered by Stimulated Raman Scattering in a simulation of a National Ignition Facility inertial fusion experiment.*  
Image credit: Eric Brugger and Steven Langer, Lawrence Livermore National Laboratory



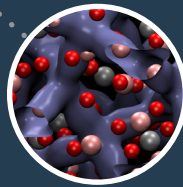
*This visualization depicts the helium mass fraction of the mixture of helium, air, and water vapor inside the PANDA containment at late time.*  
Image credit: Paul Fischer, Aleksander Obabko, and Ananias Tomboulides, Argonne National Laboratory



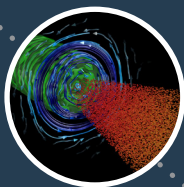
*An early design of an artificial peptide (shown in gold) intended to bind to an HIV protein to treat HIV infection.*  
Image credit: Vikram K. Mulligan, University of Washington



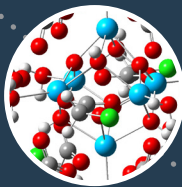
*Reactive molecular dynamics showing electric field sintering of FeOx nanoparticles to form a thin film.*  
Image credit: Subramanian Sankaranarayanan, Argonne National Laboratory



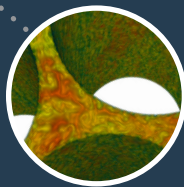
*An image of LLZO (200 atoms), a promising material for solid-state electrolytes.*  
Image credit: Alessandro Curioni and Teodoro Laino, IBM Research Zurich



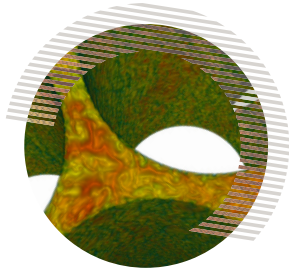
*Interaction of a fast-ignition-scale laser with a dense plasma.*  
Image credit: Frederico Fiuza, Lawrence Livermore National Laboratory



*Density functional theory-optimized structure for  $\text{Th}_6(\text{OH})_4\text{O}_4(\text{H}_2\text{O})_6(\text{C}_1\text{CH}_2\text{COO})_{12}$*   
Image credit: Karah Knope and Lynne Soderholm, Argonne National Laboratory;  
David Dixon and Monica Vasiliu, University of Alabama



*Large eddy simulation of the flow in a rod bundle at high Reynolds numbers.*  
Image credit: Elia Merzari and Justin Walker, Argonne National Laboratory



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