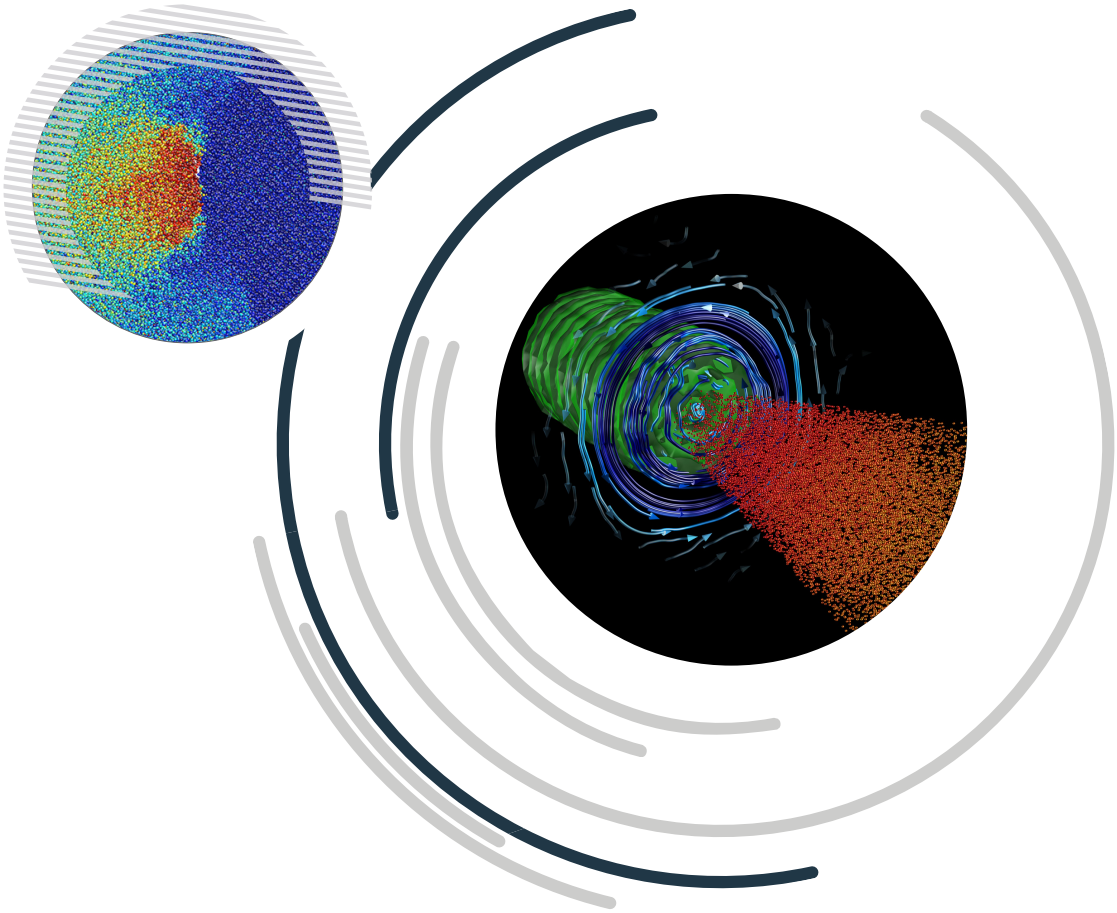
Argonne NATIONAL LABORATORY

ARGONNE **LEADERSHIP COMPUTING** FACILITY

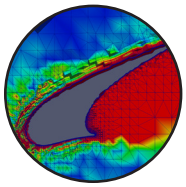
2014 **ANNUAL REPORT**



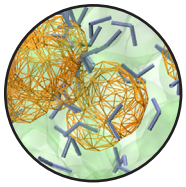
ARGONNE **LEADERSHIP COMPUTING** FACILITY

2014 **ANNUAL REPORT**

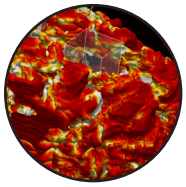
TABLE OF **CONTENTS**



ALCF YEAR IN REVIEW



EXPERTISE, RESOURCES & ALLOCATION PROGRAMS



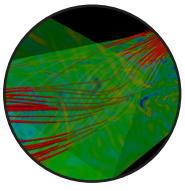
SCIENCE HIGHLIGHTS

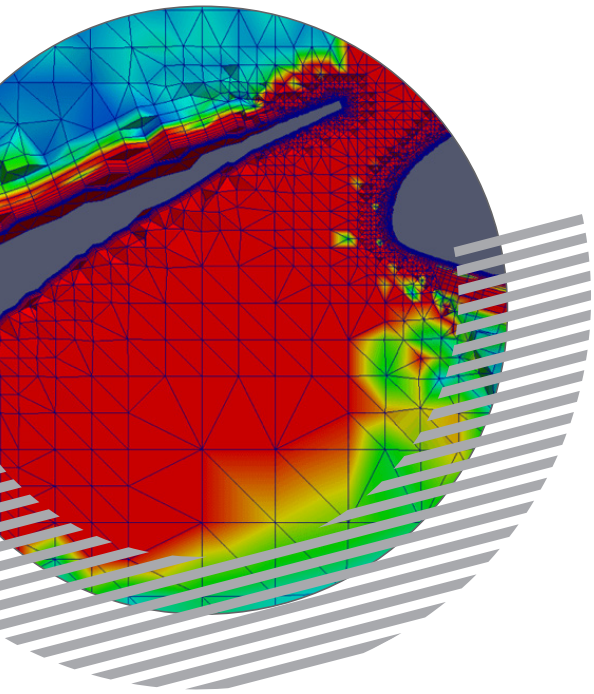
BIOLOGICAL SCIENCES

CHEMISTRY

COMPUTER SCIENCE

EARTH SCIENCE





2014 BY THE NUMBERS

5.8
billion core-hours of total compute time

342
active projects

1,432
facility users*

150+
publications

* Fiscal year 2014

ABOUT ALCF

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

Supported by the U.S. Department of Energy's Office of Science, Advanced Scientific Computing Research program, the ALCF is one half of the DOE Leadership Computing Facility, which deploys two diverse high-performance computer architectures dedicated to open science.

Available to researchers from universities, industry, and government agencies, the ALCF helps accelerate the pace of discovery and innovation by providing supercomputing resources that are 10 to 100 times more powerful than systems typically available for open scientific research.

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

DIRECTOR'S MESSAGE

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

2014 was Mira's first full "production" year, a term that describes both the technical ability and the practical utility of a high-performance computing system running at full-scale. And in 2014, once again the Argonne Leadership Computing Facility met or exceeded every one of its goals as a high-end scientific computing center.

The ALCF also delivered 5.8 billion core-hours on Mira, perhaps the most salient metric of a leadership-class facility serving the scientific and engineering research community. This number represents the cycles that enabled the individual project achievements that you will read about in the pages that follow. Mira is enabling more detailed simulations of human pathologies, aiding alternative energy research on a number of fronts, promoting the development of revolutionary new materials, and much more.

This year, we also took on the monumental task of dismantling Mira's predecessor, a 40-rack IBM Blue Gene/P supercomputer called Intrepid, donating three of its racks to North Carolina State University and recycling its remaining components. Thousands of pounds of copper and many tons of steel were salvaged. The racks that found a new home at NCSU will be used for teaching parallel programming classes and for active research.

We are now firmly focused on the future. In March, the CORAL collaboration between Oak Ridge, Argonne, and Lawrence Livermore national laboratories selected two industry partners to build and deliver the Department of Energy's next generation of leadership computers. In November, following several successful design reviews, the ALCF-3 project was given the green light to begin the final approval process for the system contract. Stay tuned for the big announcement in early 2015!

As we begin preparations for our new machine, I'd like to acknowledge the efforts of all the people who make the ALCF successful. Our outreach team is reaching and training more potential users, our computational scientists and performance engineers are enabling more effective and efficient use of our systems, our data analysis and visualization experts are finding new and interesting ways to generate insight, and our operations team is doing a fantastic job at keeping the systems and software running smoothly.

We remain aware of our important mission and hope you are as excited about our future as we are.

ALCF YEAR IN REVIEW

SUSAN COGHLAN
Deputy Director

Future Systems and Facility Initiatives

We made considerable progress in our efforts to secure DOE's next-generation leadership computing systems as part of the Collaboration of Oak Ridge, Argonne, and Livermore (CORAL). In March, as the result of a competitive request for proposals, the CORAL labs selected the vendors for their future supercomputers, which are scheduled for delivery in 2017-2018. Through successful ALCF-3 Design and CD-2/3b reviews, we fine-tuned the configuration of our system and finalized the project cost, scope, and schedule. Next year, we look forward to awarding the system contract and working with the vendor to begin the process of developing and delivering an innovative and powerful new system. Also in 2014, our Business Intelligence team continued efforts to enhance our data reporting and analysis capabilities, which have improved internal operations, trending analysis, and many other important business functions.

PAUL MESSINA
Director of Science

Science

In 2014, we supported 40 INCITE and 21 ALCC projects, indicative of the many meritorious proposals that require leadership computing resources and evidence of strong interest in Mira. We hosted and facilitated a quantum Monte Carlo workshop, sponsored by DOE's Basic Energy Sciences program and the National Science Foundation. This event was a great example of how we work closely with domain scientists to explore approaches that are well suited for today's and tomorrow's leadership computers. We also began joint application readiness and performance portability efforts with Oak Ridge Leadership Computing Facility (OLCF) and National Energy Research Scientific Computing Center (NERSC) for the next generation of DOE supercomputers. Our Early Science Program for Mira is serving as a model for OLCF and NERSC as they plan for their next systems. Our team also performed a study to analyze the scalability of 2014 INCITE projects and their approach to programming model use. The study revealed that most projects have threaded their applications, which bodes well for the transition to future systems with increased hardware concurrency per node.

BILL ALLCOCK
Director of Operations

Operations

We completed a major upgrade of the HPSS system, which improved the bandwidth and capacity of the disk cache by 4x. We also improved the resiliency and increased the capacity of the Mira file systems, while laying the groundwork for additional improvements next year that will continue to make data management easier for our users so they can focus more on science. On a sad note, we successfully decommissioned Intrepid, the very first system that ALCF fielded. Having completed its first full year of production, Mira is settling down nicely. This year, we posted our best scheduled availability ever and our second best overall availability. With several enhancements occurring over the course of the year, I am hopeful we can improve on this even further. In 2015, we will continue our storage improvements by bringing a "burst buffer-like" storage cache online and we will deploy a new visualization cluster.

RICHARD COFFEY
Director of User Experience

User Experience

We expanded our efforts in four key areas for ALCF: informing the public, finding potential users, improving the ALCF experience for new and returning users, and developing training and outreach events. The communications team generated a new set of science stories—a critical piece of our strategy to amplify the impact of our facility. These articles provide valuable success stories that ripple through DOE headquarters, Argonne's extensive media channels, and the community fostered by the ALCF. Over this last year, we rigorously evaluated and measured several key user and project processes. We built an industry outreach program to encourage more companies to use our facility. We captured 68 hours of exceptional online videos that document the entire Argonne Training Program on Extreme-Scale Computing. 2015 promises to be another exciting year of change and growth aimed at providing the very best experience for our users.

KALYAN KUMARAN
Manager, Performance Engineering

Performance Engineering

Our team provided one-on-one optimization support to ALCF users, while also working on numerous initiatives aimed at improving the future of leadership computing. We helped train and assist current and future users by participating in the ALCF's annual Mira Performance Boot Camp and Argonne Training Program on Extreme-Scale Computing. We also contributed extensively to ongoing plans for the ALCF's next supercomputer, including reviewing proposals and writing technical specifications. In addition, we partnered with Argonne's Mathematics and Computer Science division to launch the Joint Laboratory for System Evaluation (JLSE) to work collaboratively on prototype technologies for petascale and beyond. As co-lead of JLSE, I'm particularly excited that this lab gives us access to the latest hardware and software to help optimize applications and design performance tools and benchmarks for next-generation systems.

MARK HERELD
Manager, Visualization and Data Analysis

Visualization and Data Analysis

This year, we continued to work closely with ALCF users to produce visualizations that help them interpret the data from their simulation runs on Mira. As one example, we enabled INCITE project scientists to better understand the evolution of galaxy halos from their trillion-particle simulations of the distribution of dark matter in the universe by developing a new method for direct rendering of large-scale particle datasets. We worked with another INCITE team to create a visualization of blood flow in cerebral aneurysms that was honored as a finalist for Best Visualization in the SC14 Visualization Showcase. In addition, we finalized contract details for the procurement of Cooley, a new visualization and analysis platform that provides a significant performance upgrade over the ALCF's current Tukey system. As we transition our activities to Cooley next year, we look forward to having a resource that will allow our users to visualize much larger datasets.

PROPELLING THE HPC COMMUNITY

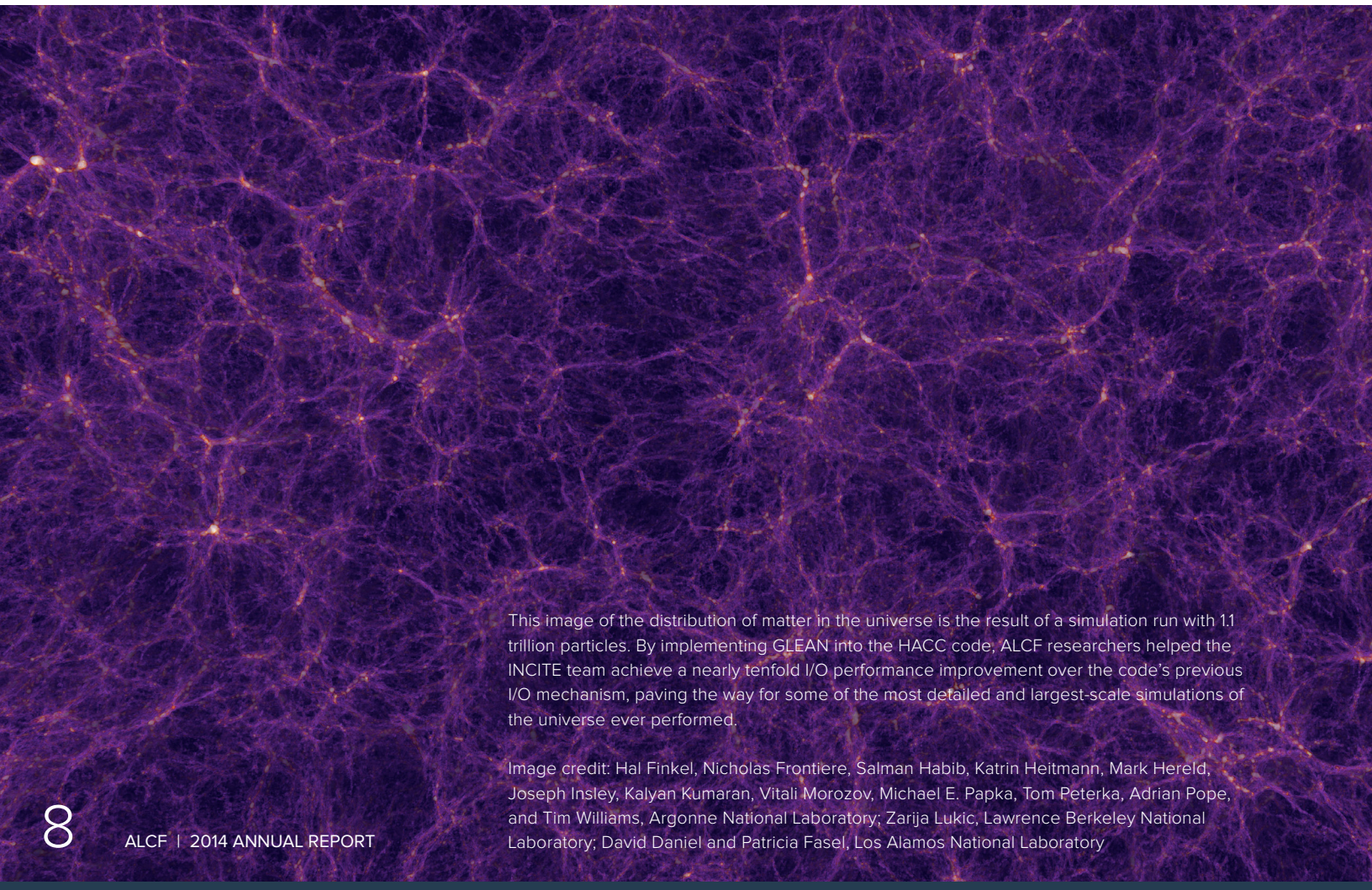
ALCF Efforts Help Shape the Future of Supercomputing

ALCF researchers are helping to develop the software, standards, and benchmarks needed to drive continued improvements in supercomputing performance, which in turn helps scientists to accelerate the pace of discovery and innovation.

With the rapid evolution of high-performance computing (HPC) systems, these efforts are crucial to enabling researchers to exploit the full scale and capability of leadership-class supercomputers.

The ALCF is committed to providing its users with a stable, effective, and innovative software environment that helps bridge the gap between leading-edge hardware and its potential for producing groundbreaking scientific results.

Working closely with the scientists who use leadership computing resources gives ALCF researchers a unique perspective on the software features and capabilities that are needed to continue pushing the boundaries of what is possible in computational science and engineering.



This image of the distribution of matter in the universe is the result of a simulation run with 1.1 trillion particles. By implementing GLEAN into the HACC code, ALCF researchers helped the INCITE team achieve a nearly tenfold I/O performance improvement over the code's previous I/O mechanism, paving the way for some of the most detailed and largest-scale simulations of the universe ever performed.

Image credit: Hal Finkel, Nicholas Frontiere, Salman Habib, Katrin Heitmann, Mark Hereld, Joseph Insley, Kalyan Kumaran, Vitali Morozov, Michael E. Papka, Tom Peterka, Adrian Pope, and Tim Williams, Argonne National Laboratory; Zarija Lukic, Lawrence Berkeley National Laboratory; David Daniel and Patricia Fasel, Los Alamos National Laboratory

ALCF performance engineer Ray Loy works with a researcher at the Mira Performance Boot Camp.

SOFTWARE INNOVATIONS

Novel software tools and techniques help users harness more processing power, accelerate the speed of calculations, improve I/O performance, and enable many other performance-related enhancements.

ASCR Collaboration to Improve Applications Portability

ALCF, OLCF, and NERSC 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 is intended to better understand the needs of users, improve application portability, and increase user participation across all facility designs.

GLEAN

ALCF researchers are developing an open source software tool, called GLEAN, to help users optimize data movement between the compute, analysis, and storage resources of HPC systems. GLEAN helps to improve I/O performance by exploiting the network topology for collective I/O, leveraging data semantics of applications, and incorporating asynchronous data staging. GLEAN can also be used to perform *in situ* analysis during large-scale simulation runs, which allows researchers to analyze data in real time.

LLVM Compiler Infrastructure

The ALCF continued making major contributions to the LLVM compiler infrastructure project this year. This included adding the ability to represent pointer aliasing information, and preserve that information as programs are optimized. The ALCF also made it possible for LLVM to provide auxiliary 'assumptions' to the optimizer to produce faster code. The improvements have been made available to ALCF users on Mira as part of the bgclang project. In addition, the ALCF continued to maintain LLVM's PowerPC backend, and improved various other aspects of the compiler.

HPC Performance Tools

The ALCF regularly collaborates with tool development groups to enhance the capabilities, scale, and reliability of various performance tools on leadership-scale systems. A recent highlight is the development of the OMPT OpenMP profiling interface, which has been published as an OpenMP Technical Report and implemented in prototype form in IBM compilers and in the TAU and HPCToolkit performance tools.

SKOPE

Developed at the ALCF, SKOPE (SKeleton for wOrkload Performance Exploration) is a performance analysis, tuning, and projection framework that helps researchers model and explore a workload's current and potential behavior. This information can play an important role in the design and adoption of new algorithms and hardware. SKOPE has become an integral tool for all stages of the ALCF life cycle. It can be used to evaluate the performance of perspective systems in procurement processes, as well as to enable performance tuning and application transformations during the production phase of ALCF systems.

Debugging Tools

Using Allinea DDT software, the ALCF performed large-scale debugging sessions to improve system resilience on Mira. Because the memory available for debugging sessions was less than anticipated, ALCF researchers put safeguards in place to prevent system impact when memory is exceeded, and worked with Allinea staff to reduce memory use further. Support for Allinea DDT was also extended to Tukey, the ALCF visualization and data cluster, allowing debugging of parallel codes, including those using GPU kernels.

BENCHMARKS

Benchmarks are required to measure and improve the performance of both systems and applications. By mimicking real-world workloads to assess memory, processor speed, interconnect performance, and other characteristics, industry-standard benchmarks are a key tool for helping applications developers achieve optimal performance.

SPEC HPG Benchmarks

The ALCF is a longtime contributor to the Standard Performance Evaluation Corporation (SPEC), a non-profit organization formed to establish, maintain, and endorse a standardized set of benchmarks that can be applied to the newest generation of HPC systems. As part of SPEC's High-Performance Group, ALCF researchers play a leadership role in developing standard application benchmarks in various programming models, including MPI, OpenMP, OpenACC, and OpenCL. Some of these benchmarks have been used in the evaluation and acceptance of ALCF supercomputers.

MPI Benchmarks

The ALCF MPI Benchmark Suite is designed to better understand the communication behavior of the hardware systems and to guide the performance tuning of scientific applications. ALCF researchers frequently update the suite with communication patterns and use-cases extracted from real applications running on ALCF computing resources. The MPI-based suite is one of the major benchmarks used in acceptance testing and helps the ALCF to ensure that its computing resources are being used efficiently. Results from the benchmarks provide important lessons learned and guide best practices for application developers and performance engineers.

Data-Centric Benchmarks

The ALCF has developed a suite of data-centric benchmarks to represent the emerging data-intensive workloads, which are of increasing importance to DOE and are becoming an integral part of many computational science domains, including cosmology, engineering, combustion, and astrophysics. These benchmarks help to assess the performance of the architecture integer operations, specifically for hashing and for memory-intensive genomics applications. The benchmarks are being used to evaluate the data-centric capabilities of the DOE's next-generation supercomputers.

STANDARDS DEVELOPMENT

The development of industry standards for programming models and interfaces, such as OpenMP and MPI, and for programming languages, such as C++, drive the development of modern applications that perform well and are portable across different hardware architectures. These standards provide a path for developing massively parallel programs in this complex and ever-changing landscape.

C++ Standards

The ALCF continued its participation in furthering the development of the C++ programming language standard and several associated technical specifications. In collaboration with several C++ compiler vendors, the ALCF has proposed an extension for providing additional pointer aliasing information to the compiler's optimizer. This feature is expected to lead to the creation of higher performance C++ scientific programs.

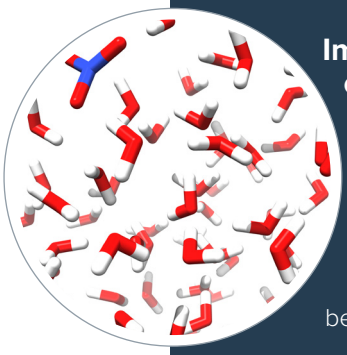
OpenMP Enhancements

The ALCF participates in the OpenMP Language Committee's continuing efforts to enhance OpenMP specifications. Several important features are currently proposed for OpenMP 4.1, including the refinement of device constructs, new extensions to handle dependencies within loops, and the creation of tasks from loops. The ALCF also participates in the OpenMP Architecture Review Board and is involved in planning for OpenMP 5.0.

From left, ALCF researchers Vitali Morozov, Kalyan Kumaran, Kevin Harms, and Tim Williams put their parallel coding skills on display as the Linear Scalers team in the Intel Parallel Universe Computing Challenge at SC14 (Hal Finkel is not pictured).

ADVANCING CODES FOR SCIENCE

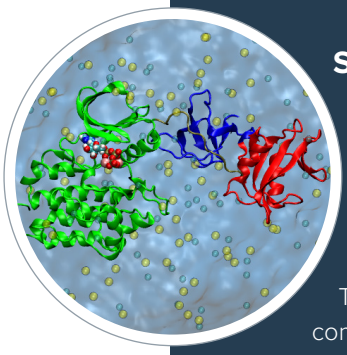
ALCF researchers contribute to the optimization and scaling of codes and algorithms to improve simulations of everything from battery materials to proteins. These code enhancements benefit the entire user community.



Implementing RATTLE in GAMESS

Code: GAMESS, an *ab initio* molecular quantum chemistry package maintained at Iowa State University, supports major quantum mechanical methods, such as density functional theory, Hartree-Fock, and coupled cluster theory.

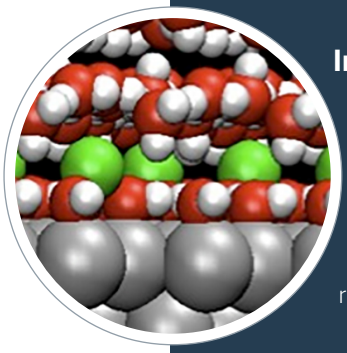
ALCF Contribution: Implemented constraint algorithm RATTLE to improve the speed and energy conservation of GAMESS. This enhancement has improved performance on Mira by allowing fewer, larger, and more efficient time steps to be taken.



Scalable Multiple-Copy Algorithms for NAMD

Code: NAMD, a parallel, object-oriented molecular dynamics from the University of Illinois at Urbana-Champaign, is designed for high-performance simulations of large biomolecular systems.

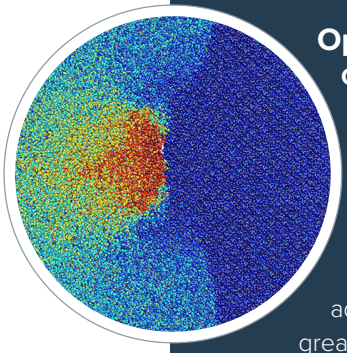
ALCF Contribution: Developed and implemented generalized multiple-copy algorithms in NAMD for accelerating sampling on top of Charm++. This improvement also gives users great flexibility in using novel solutions for complex biophysical problems without having to modify the source code.



Improving the Performance of QMCPACK

Code: Developed at University of Illinois at Urbana-Champaign, QMCPACK is a production-level many-body quantum Monte Carlo code used to compute the electronic structure of atoms, molecules, and solids.

ALCF Contribution: Improved the performance of QMCPACK using QPX intrinsics, L1 prefetcher, and other loop-based optimization. These efforts have resulted in a 2x speedup on Mira.



Optimizations to LAMMPS

Code: LAMMPS, a classical molecular dynamics code from Sandia National Laboratories, can be used to model solid-state materials (metals, semiconductors), soft matter (biomolecules, polymers), and coarse-grained or mesoscopic systems.

ALCF Contribution (in collaboration with IBM): Rewrote the PPPM electrostatic solver to use MPI collectives, optimized OpenMP threading, and added support for MPI-I/O. These efforts have resulted in a 4x speedup in I/O, a greater than 2x speedup in the overall performance of LAMMPS, and improvements to the MPICH MPI-I/O source code.

PARTNERING WITH INDUSTRY FOR HIGH-IMPACT RESEARCH

High-performance computing is a powerful tool for driving innovation and competitiveness in the private sector.

With faster computers and more sophisticated software, companies can tackle more complex problems, achieve more accurate predictions, and create higher fidelity models of everything from combustion to battery materials.

As a DOE Office of Science User Facility with supercomputing resources that are significantly more powerful than typical research computing systems, the ALCF has the hardware, as well as the expertise, to enable modeling and simulation campaigns that can accelerate research and development efforts for many industry applications.

With the potential for immediate commercial impacts, industry projects are an important component of the ALCF user community. Through communication and outreach efforts, ALCF seeks to grow its base of industry users by identifying prospective companies that could benefit from leadership computing resources and facilitating opportunities for collaboration with ALCF and across Argonne.

Background image: Noise generation due to turbulent mixing of exhaust flow. Large eddy simulation of exhaust flow from a two-inch conic nozzle with exit Mach number of 0.97. Visualizing density gradients in the flow. Image credit: Joseph Insley, Argonne National Laboratory; Umesh Paliath, GE Global Research.

More Energy-Efficient Technologies

GE Global Research is using an INCITE award to study the complex physics of combustor liner flows to help engineers develop aircraft engines with better fuel efficiency, lower emissions, and improved performance. GE researchers have also used ALCF supercomputers in recent years to investigate ways to decrease jet engine noise and improve the efficiency of wind turbines.

Next-Generation Aircraft Design

Boeing has used ALCF supercomputers to simulate the turbulence and noise created by aircraft landing gear to contribute to the design of next-generation aviation technologies. In 2015, Boeing will use a new INCITE award to simulate the complex turbulent flows that occur on aircraft wings, providing data to improve turbulence models used in aircraft design.

Oil Platform Safety

With an INCITE award, researchers from CERFACS are using Mira to study the mechanics of flame and explosion propagation in confined spaces. Energy company Total is partnering with the researchers due to interest in mitigating the potential of accidental explosions on offshore oil platforms.

Engine Modeling and Simulation

Through Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI), a multidisciplinary team is collaborating with Caterpillar and Convergent Science Inc. to develop engine modeling and simulation capabilities for Mira and other high-performance computers to aid in the design of next-generation engines. With a Director's Discretionary award at the ALCF, they are working to optimize and improve the scalability of CONVERGE, a computational fluid dynamics code widely used in the automotive industry.

Drug Design and Development

Cloud Pharmaceuticals, a North Carolina-based company focused on cloud-based drug design and development, is using Mira through a Director's Discretionary award to identify leading drug candidates for broad-impact, anti-parasitic therapeutics targeting several orphan diseases including malaria.

ALCF hosts students from the Science Careers in Search of Women conference.

GROWING THE HPC COMMUNITY

ALCF Education and Outreach Activities Strengthen the Future of Leadership Computing

The ALCF is actively engaged in training and outreach efforts to educate computational scientists and engineers on best practices and new trends, while also aiming to grow the high-performance computing (HPC) user community and workforce of tomorrow.

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

Inspiring Young Minds

Outreach efforts begin at the middle school and high school level with activities aimed at highlighting the exciting science enabled by supercomputers. Through ALCF participation in Argonne events like Introduce a Girl to Engineering Day and the Science Careers in Search of Women conference, young students are able to learn about supercomputing firsthand and to see how they could possibly fit into this emerging field.

Students from the Notre Dame Summer Scholars program visit the ALCF machine room.

Guided facility tours are another educational tool used to introduce students to Mira and the groundbreaking research being conducted at the ALCF. In July, for example, the ALCF hosted a group of high school students from the Notre Dame Summer Scholars program focused on research computing.

"Learning about Mira and HPC capabilities at the highest echelon was a capstone part of our two-week program on scientific computing," said Paul Brenner, associate director of Notre Dame's Center for Research Computing. "Our visit to the ALCF helped inspire a new generation of scientists and engineers to use supercomputers to answer our society's complex challenges."

A Launching Pad for Careers in HPC

Each year, the ALCF employs several students and postdocs, providing them with a unique opportunity to work at the forefront of scientific computing.

With 20 college students taking part in the ALCF's summer student program this year, it was the facility's largest group to date. The students were paired with mentors in practically every area of the ALCF, from visualization and performance engineering to computational science and industry outreach. The 10-week program culminated with a special seminar that allowed the students to present their project results.

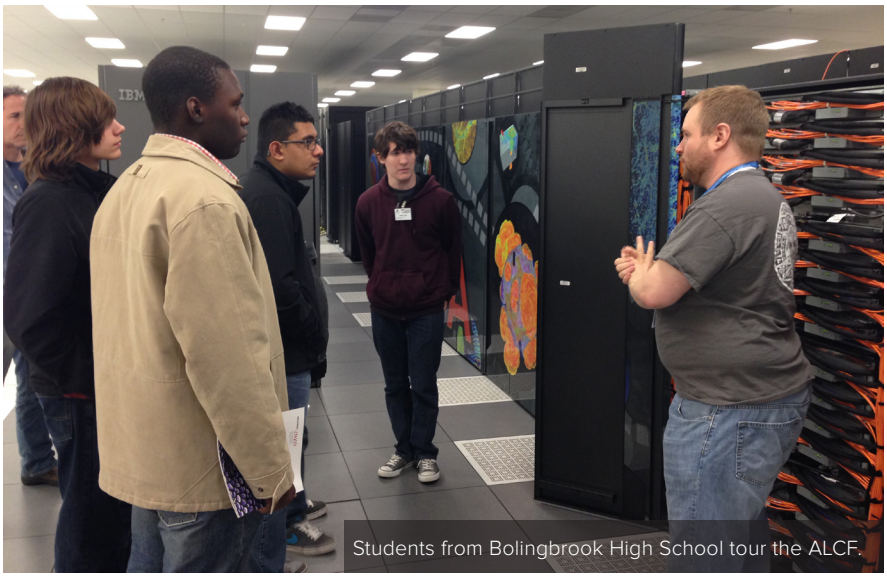
In 2014, the ALCF also launched the Margaret Butler Fellowship to commemorate a pioneering woman and scientist in both computer science and nuclear energy. The fellowship was created to give postdoctoral candidates an opportunity to collaborate with Argonne scientists to use Mira to push scientific boundaries in their field of expertise. Ying Li, a postdoc from University of Southern California, joined the ALCF this fall as the first recipient of the fellowship.

Training Computational Scientists

The ALCF makes it a priority to educate current and future users by offering several expert-guided, hands-on training opportunities to inform them of the tools, computational resources, and services available to them in support of scientific discovery.

The Argonne Training Program on Extreme-Scale Computing (ATPESC) is one of the most intensive HPC training programs in the world. Conceived and organized by ALCF Director of Science Paul Messina and funded by the DOE's Office of Science, ATPESC brings in about 60 students each year for a 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.

"Systems like Mira can enable breakthroughs in science, but to use them productively requires


Students from Bolingbrook High School tour the ALCF.


ATPESC 2014


Mira Performance Boot Camp

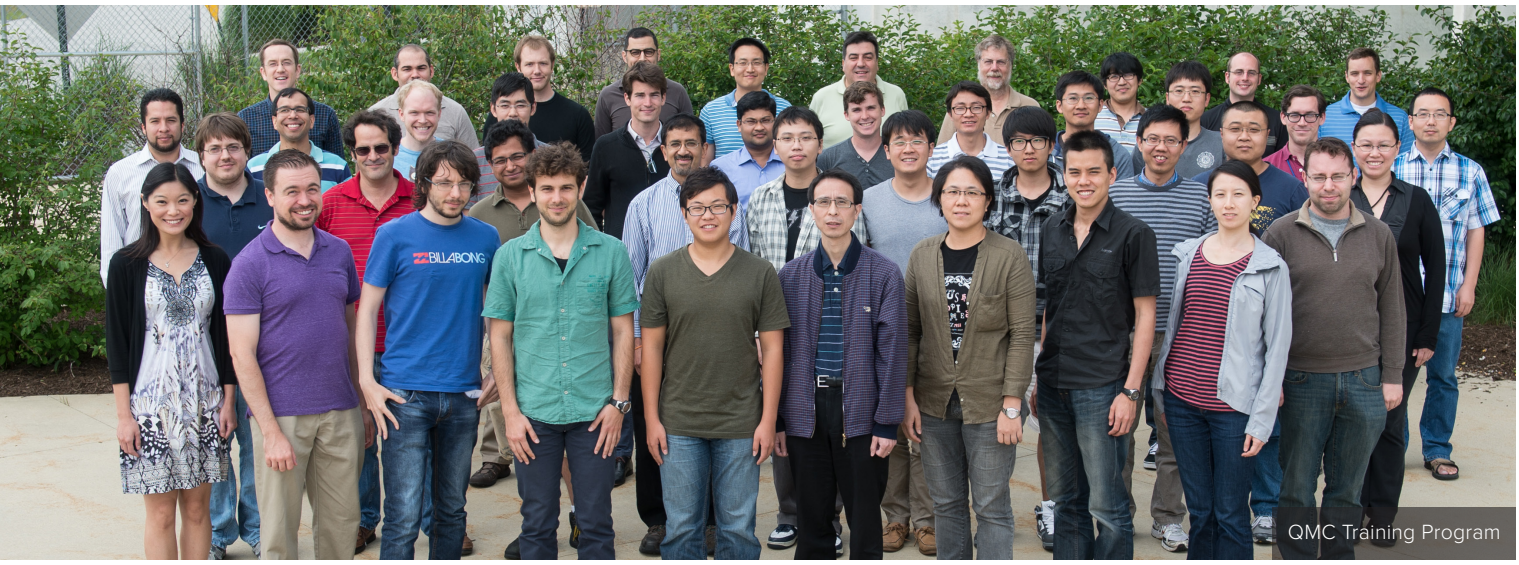
significant expertise in a number of disciplines. Our training program exposes the participants to those topics and provides hands-on exercises for experimenting with most of them," Messina said. With videos of the past ATPESC lectures available online, the program's reach has been extended beyond the classroom as well.

As another example of advanced training, the ALCF hosted a workshop on quantum Monte Carlo (QMC), an increasingly popular computational method for chemistry, materials science, and physics research.

Designed to expand the user base of QMC, the weeklong program, which was supported by the DOE Office of Science and the National Science Foundation, brought in 33 participants consisting of scientists, professors, and graduate students.

The workshop 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.

In addition to these special training programs, the ALCF also puts on annual events to ensure its users make the most of their computing time at the facility. For example, the Mira Performance Boot Camp gives researchers a chance to work directly with ALCF staff to improve their code's scalability to demonstrate computational readiness for a future INCITE award, while interactive Getting Started videoconferences provide new users with everything they need to know to begin using ALCF services and resources.



QMC Training Program

ALCF SPONSORS TEAM IN SC14 STUDENT CLUSTER CHALLENGE

As the sponsor of an SC14 Student Cluster Challenge team, the ALCF helped provide the ultimate hands-on learning experience to a group of six students interested in high-performance computing.

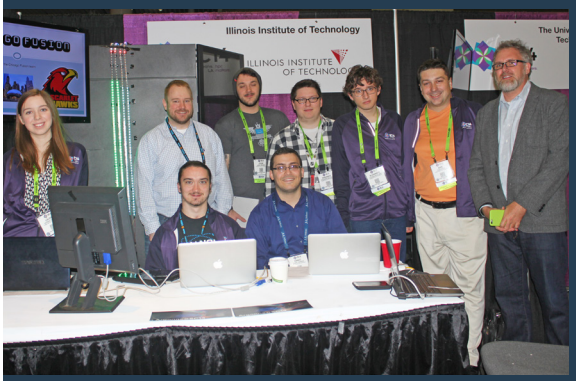
At SC14 in New Orleans, the students were one of 12 teams given 48 hours to assemble a working cluster on the conference exhibit floor and demonstrate its performance using real scientific applications and benchmarks.

ALCF staff work with the Chicago Fusion team at SC14.

With funding and technical support provided by the ALCF, the Chicago Fusion team, comprised of five college students from the Illinois Institute of Technology (IIT) and one high school senior from Glenbrook South High School, built an eight-node cluster valued at more than $250,000. The team took home the award for highest unmodified LINPACK performance (a widely used benchmark in high-performance computing).

ALCF researchers Ben Allen and William Scullin worked closely with the students to provide logistical, setup, and application support. ALCF Director Michael Papka facilitated the sponsorship, allocating staff and computing resources to the project.

Prior to SC14, the team spent months preparing to design and build the cluster. Allen and Scullin worked directly with vendors to secure the necessary computing equipment. Once the hardware arrived, they helped the students assemble the servers and wire the networking and power in a safe manner. The ALCF mentors also provided guidance on the use of provisioning tools and the applications that were part of the competition. Wanda Woods, ALCF budget and resource administrator, provided additional support, overseeing hardware orders and shipping components to New Orleans and back.



The Chicago Fusion team at SC14 in New Orleans. Standing, from left to right: Lauren Ribordy (Glenbrook South High School), William Scullin (ALCF), Jason DiBabbo (IIT), Ben Walters (IIT), Alex Ballmer (IIT), Ioan Raicu (IIT/Argonne), and Michael Papka (ALCF). Seated, from left to right: Kevin Brandstatter (IIT) and Daniel Gordon (IIT).

"The students worked really hard from June to November, investing over 2,500 collective hours preparing and participating in this competition on the world stage," said Chicago Fusion coach Ioan Raicu, an assistant professor at IIT and a guest research faculty at Argonne. "Our participation in this event would not have been possible without the support provided by the ALCF."

INCREASING AWARENESS ON CAPITOL HILL

To increase awareness of the value of leadership computing, the ALCF regularly participates in events and conferences to communicate how the facility's unique capabilities and expertise are critical to addressing some of our nation's most pressing science and engineering challenges. In 2014, this included two events on Capitol Hill aimed at Congress.

In July, the ALCF collaborated with the Oak Ridge Leadership Computing Facility to highlight leadership computing at the National User Facility Organization's annual science exhibition. The joint display covered the basics of parallel computing, presented examples of impactful research projects, and provided a real-time look at the simulations running on Mira.

ALCF staff also helped facilitate an HPC exhibit at the DOE's first-ever National Lab Day, a September event that showcased the impact of the national lab system in advancing U.S. competitiveness and innovation. The interactive HPC display featured scientific visualizations and notable accomplishments enabled by DOE computing resources.

At the National User Forum Organization's science exhibition, David Martin, ALCF industrial outreach lead, explains how researchers from University of Colorado Boulder are using Mira to improve the aerodynamic performance of airplane wings.

Interactive touch-screen displays at National Lab Day allowed Congress and members of the public to learn about the fascinating research being done at Argonne and other national laboratories.

Fuel injection and droplet breakup in a complex geometry combustor.

Image credit: Cascade Technologies

LEADERSHIP IN COMPUTING

The term “leadership” does not just apply to the ALCF’s powerful computing resources. It also applies to the people working to support facility users and maintain ALCF machines.

PAUL MESSINA

Argonne Distinguished Fellow

In 2014, Paul Messina, ALCF Director of Science, was named an Argonne National Laboratory Distinguished Fellow, the laboratory’s highest scientific and engineering rank. A true pioneer in the high-performance computing community, Paul’s storied career has involved designing, directing, and executing numerous initiatives that have influenced U.S. policy and programs related to scientific computing. At the ALCF, Paul has been instrumental in the government’s planning efforts to develop an exascale system, organizing workshops on behalf of the DOE’s Advanced Scientific Computing Research program to identify the potential scientific and national security benefits of future systems, as well as the technical challenges that must be met. Since 2013, Paul has directed the Argonne Training Program on Extreme-Scale Computing, a two-week intensive training course aimed at preparing the next generation of supercomputer users.

JINI RAMPRAKASH

Leading by Example

Jini Ramprakash leads a team of user experience analysts in providing support to researchers across the world, ensuring the experience of using Mira is as smooth as possible. She also helped launch the ALCF’s business intelligence efforts to improve data reporting for internal and external stakeholders. In addition to driving key efforts at the ALCF, Jini is passionate about encouraging more girls and young women to take a similar path toward careers in STEM (Science, Technology, Engineering, and Mathematics). She regularly participates in and helps organize Argonne initiatives to inspire young women to enter these fields, including Introduce a Girl to Engineering Day, Science Careers in Search of Women, and the Women in Science and Technology program. She is also a fixture at the annual Grace Hopper Celebration of Women in Computing Conference. With a leadership position at a DOE national laboratory, Jini serves as an inspiration for the many young women she mentors and interacts with each year.

JOSEPH INSLEY

From Simulation to Visualization

With a background in visual arts and computer science, Joe Insley brings a unique perspective and aesthetic to scientific visualizations. As one of the ALCF’s in-house visualization experts, he collaborates with INCITE researchers and other ALCF users to convert simulation data into stunning images and animations that provide new insights into complex science and engineering problems. This year, Joe’s work on a blood flow visualization was a finalist for Best Visualization in the SC14 Visualization Showcase. He also shared his knowledge of visualization and data analysis with current and future HPC users as a presenter at many ALCF-sponsored events, including the Argonne Training Program on Extreme-Scale Computing, Mira Performance Boot Camp, and a Getting Started with ParaView video tutorial.

With a shared passion for research and innovation, the ALCF's talented and diverse staff help make the facility one of the world's premier centers for computational science and engineering.

YING LI

Inaugural Margaret Butler Fellow

Ying Li joined the ALCF in 2014 as the first recipient of the Margaret Butler Postdoctoral Fellow. Ying recently graduated from the University of Southern California with a doctorate in materials science and a master's degree in computer science. As a member of a prominent computational materials science research team led by USC professor Priya Vashishta, she has already worked on massively parallel computers, including Mira, in several investigations involving reactive force-field molecular dynamics simulations of 100 million atoms. At the ALCF, she is helping to advance materials science codes for high-performance computers. Ying is also collaborating with scientists to use Mira to explore the mesostructure of silicon carbide oxide products for self-healing materials and the surface reaction of electrolytes near the cathode/anode for advanced battery materials.

RAY LOY

Preparing for Next-Generation Supercomputers

As an applications performance engineer at the ALCF, Ray Loy's typical day can involve anything from investigating code performance issues to assisting with parallel debugging. In 2014, he played a key role in helping the ALCF prepare for its next supercomputer as a member of the technical evaluation team that reviewed proposals for the next-generation system and the session lead for system software. Ray is also member of the ALCF's application readiness team, working to prepare scientific applications for future leadership-class machines. Outside of the ALCF, Ray is a member of the OpenMP Language Committee and also serves as the chair of ScicomP, the IBM HPC Systems Scientific Computing User Group. This year, he helped organize ScicomP's annual meeting in Chicago, which brought scientists, engineers, and IBM staff together to share lessons learned and best practices in porting, tuning, and running codes on IBM supercomputers.

HAL FINKEL

Simulating the Cosmos

Hal Finkel got his start in high-performance computing as a scholar in the DOE Computational Science Graduate Fellowship program and then as a postdoc in the ALCF's Early Science Program for Mira. In his current role as assistant computational scientist at the ALCF, he works closely with physics-related INCITE projects, including Argonne scientist Salman Habib's ongoing cosmology research. In 2014, Hal's solver optimization efforts helped Habib's team complete the largest high-resolution cosmological simulation ever performed. He is also the lead developer of bgclang, an open source C/C++ compiler for Mira and other supercomputers, which enables a number of projects running on ALCF computing resources. On top of all this, Hal is also active in the development of standards for the C++ programming language.

ALCF EXPERTISE

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

68 staff members

12 postdocs

20 summer students

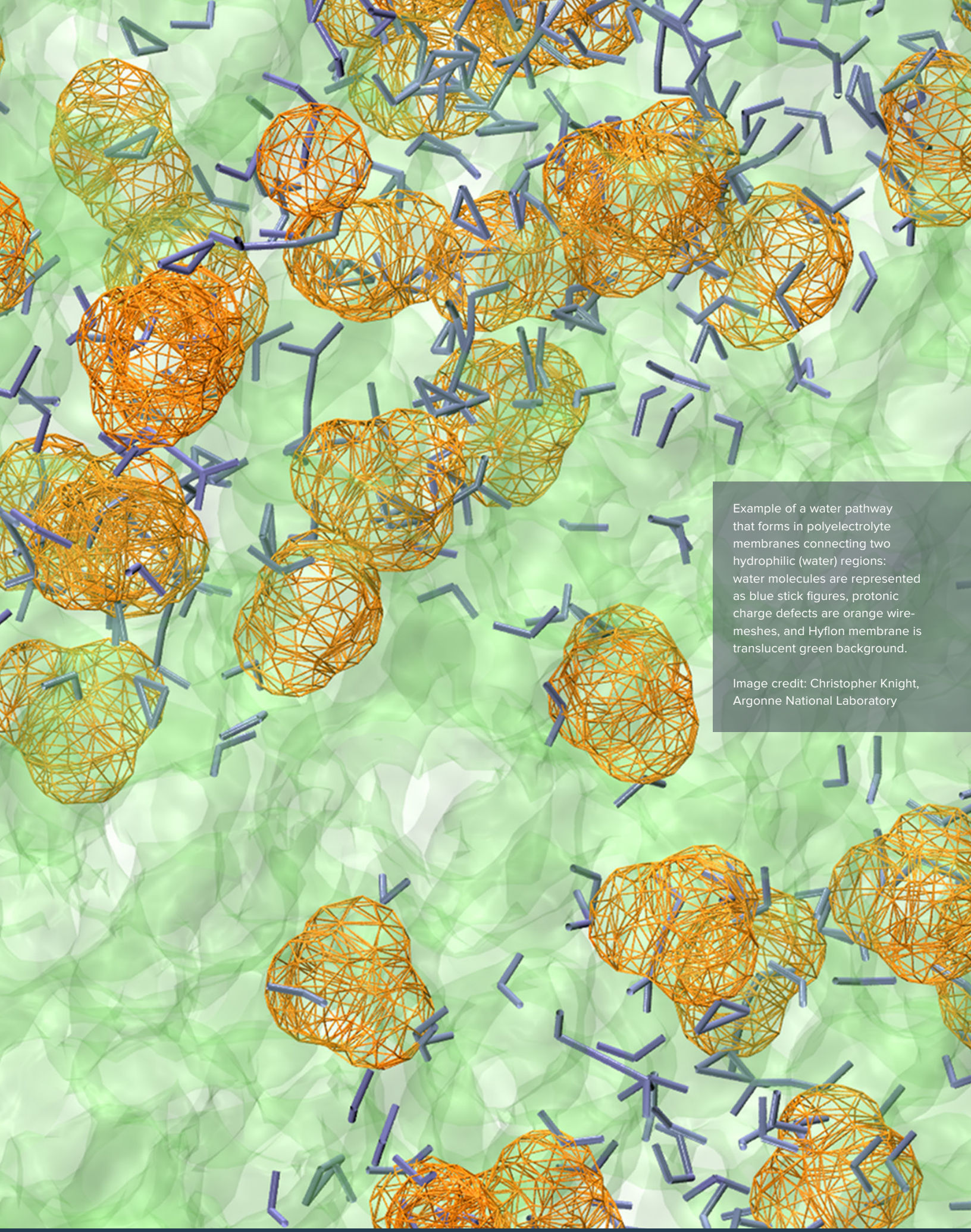
Catalysts are computational scientists who work directly with project teams to maximize and accelerate their research efforts. With multidisciplinary domain expertise, a deep knowledge of the ALCF computing environment, and experience with programming methods and community codes, the catalyst team helps users surmount any obstacles they may encounter using ALCF computing resources. This includes recruiting and collaborating with colleagues from other ALCF teams to resolve issues when additional expertise is required.

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.

Performance Engineers help users achieve optimal performance on ALCF resources by working with them to port, tune, and parallelize scientific applications and other software on current and emerging systems. The team also helps drive the future of high-performance computing and data-intensive computing through research and development of performance models and scalable algorithms, and the development of standards for key areas such as benchmarks, compilers, and programming models.

User Experience coordinates communications, support, and outreach for the ALCF. The communications team stewards ALCF user stories and ensures that the facility provides relevant and accurate information to users, DOE, and the public at large. The support team manages the workflows for user accounts and projects, and assists users with support requests related to their ALCF projects. Outreach focuses on organizing training efforts and user-centered events for the ALCF.



Example of a water pathway that forms in polyelectrolyte membranes connecting two hydrophilic (water) regions: water molecules are represented as blue stick figures, protonic charge defects are orange wire-meshes, and Hyflon membrane is translucent green background.

Image credit: Christopher Knight, Argonne National Laboratory

COMPUTING RESOURCES

MIRA

Mira, the ALCF's 10-petaflops IBM Blue Gene/Q 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

16 — 1600 MHz PowerPC A2 CORES Per Node

RACKS — 48

49,152 — NODES

CORES — 786,432

16 GB — RAM Per Node

TORUS Interconnect — 5D

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 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 RAM

The full Tukey system has:

- 96 nodes
- 1,536 cores
- QDR InfiniBand interconnect
- 6 TiB RAM
- 1.1 TiB 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.

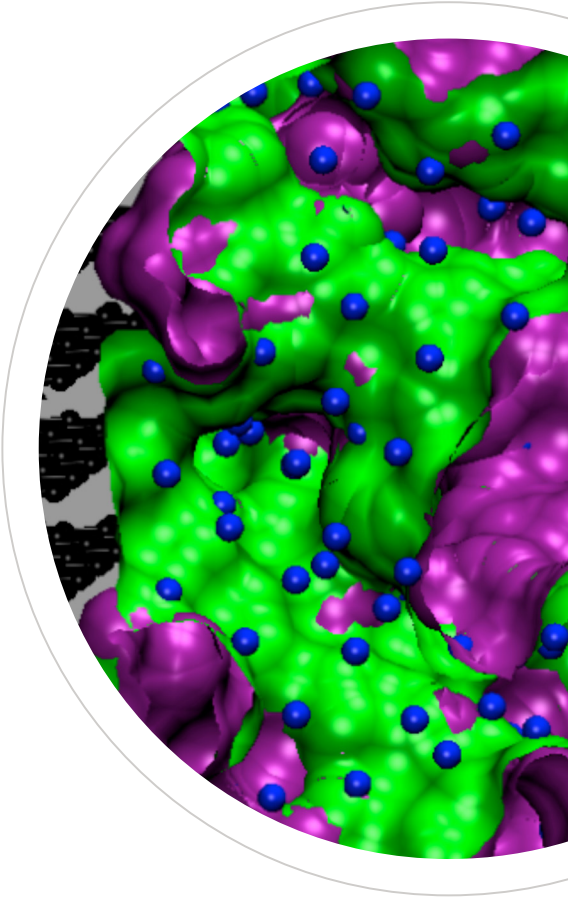
Disk Storage: The Blue Gene/Q data systems consist of 384 I/O nodes that connect to 22 storage arrays that control 13,000 disk drives with a total useable capacity of 27 PB and a maximum aggregate transfer speed of 330 GB/s over two file systems. The ALCF uses the GPFS file system to access the storage.

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.



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)

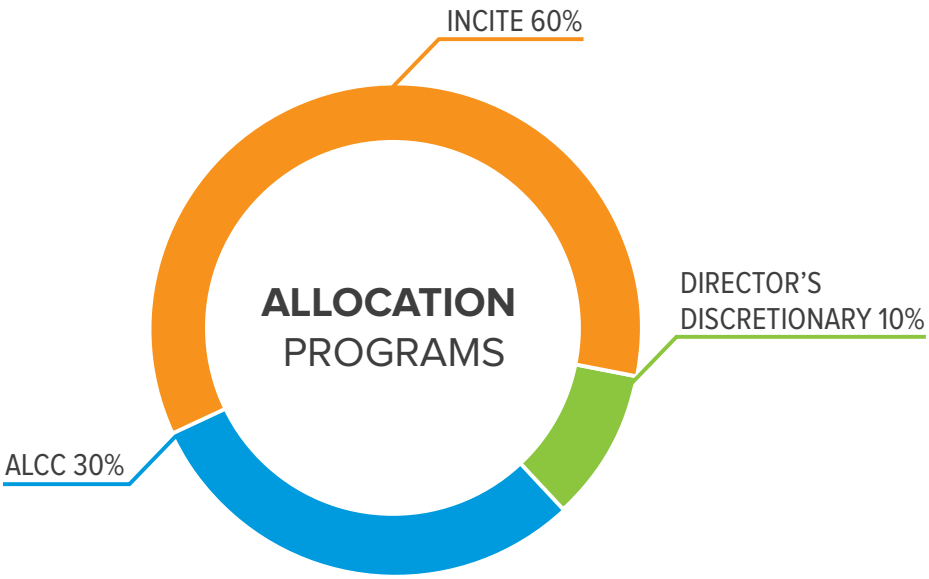
The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering. The program conducts a two-part review of all proposals: a peer review by an international panel of experts and a computational-readiness 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)

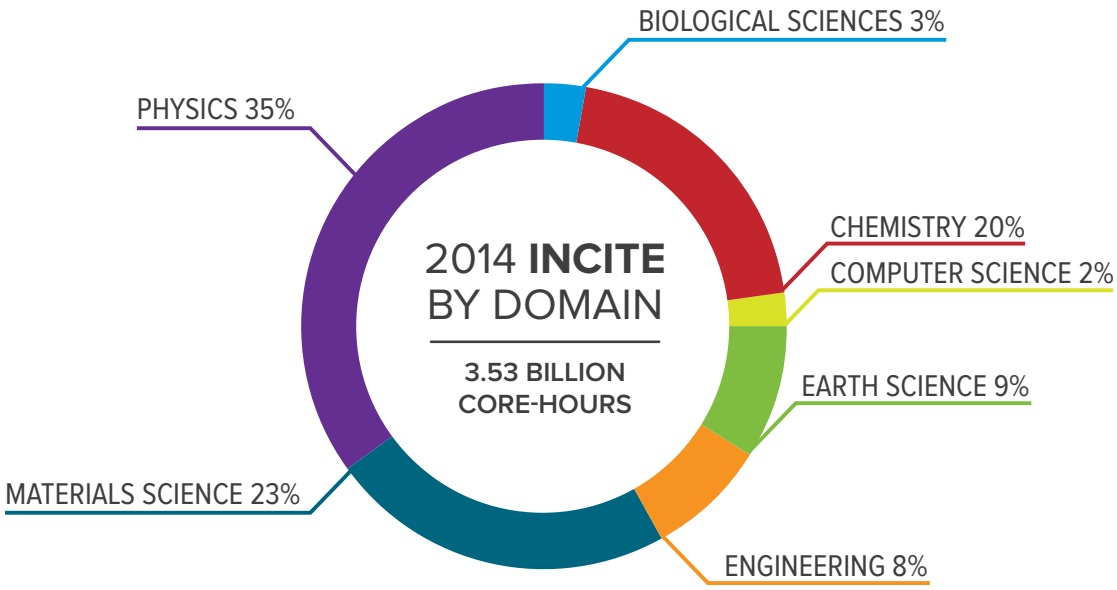
The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources. The DOE conducts a peer review of all proposals based on scientific and technical 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.

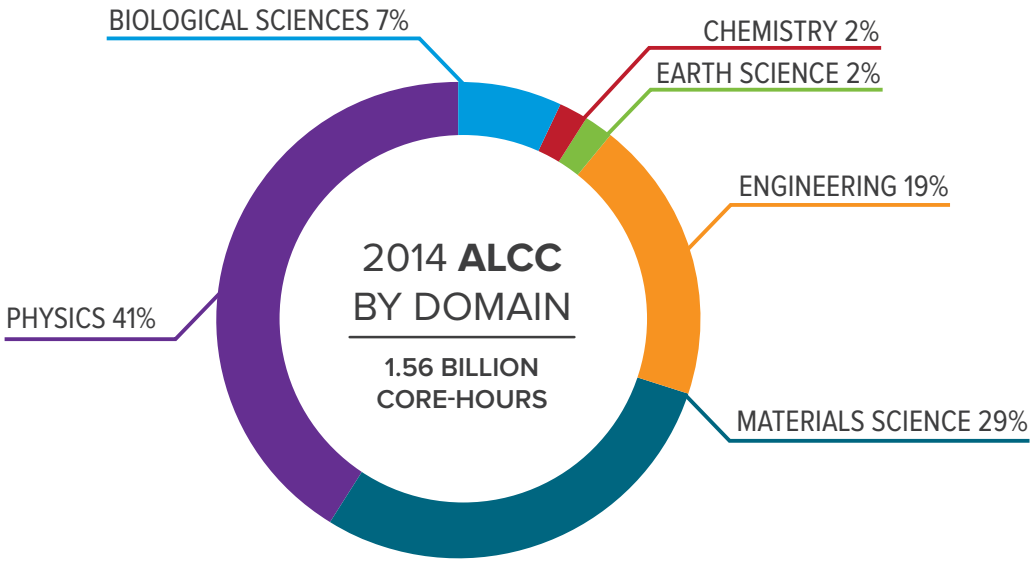
Director's Discretionary (DD)

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.

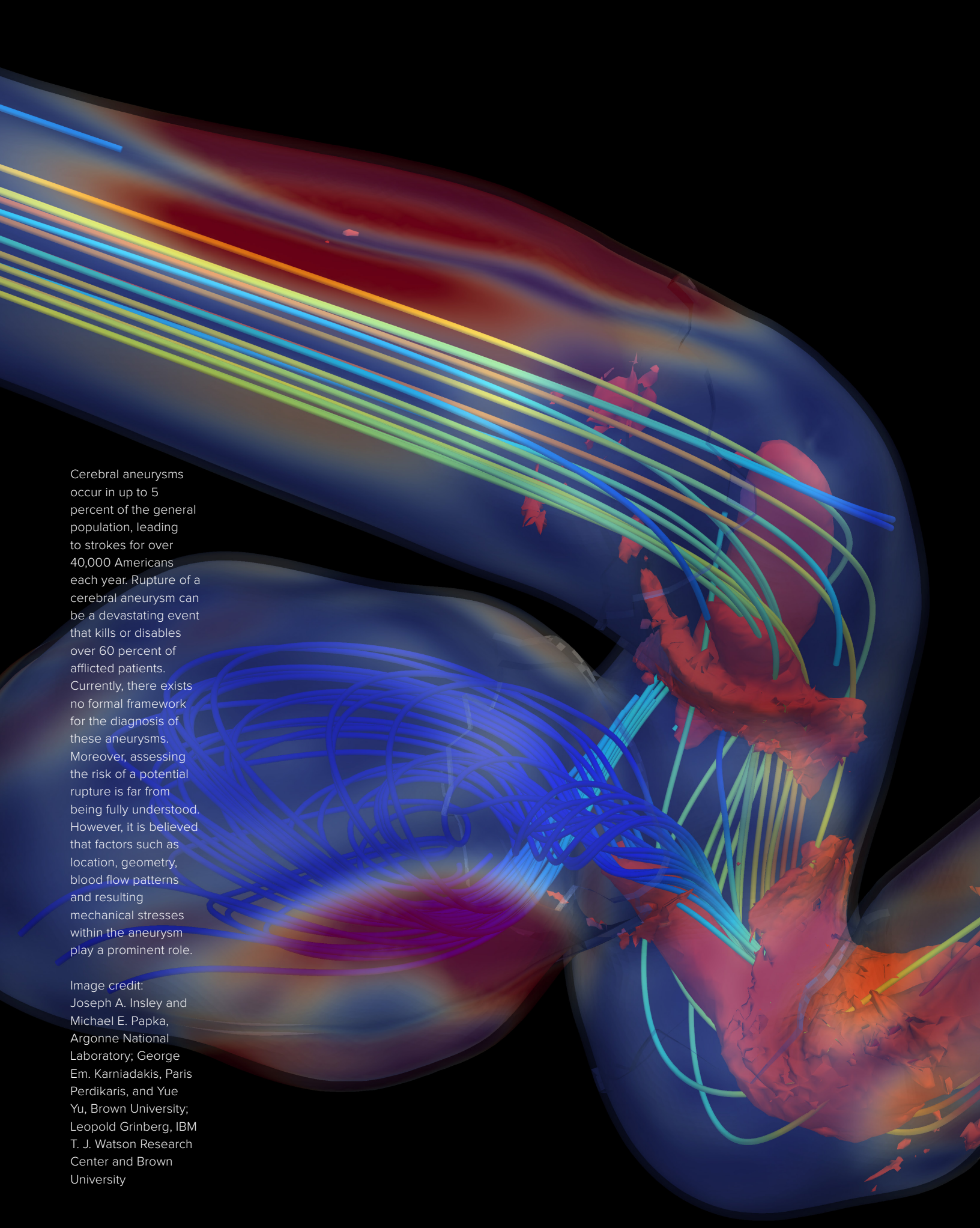


A breakdown of how ALCF computing time is allotted among the three allocation programs.





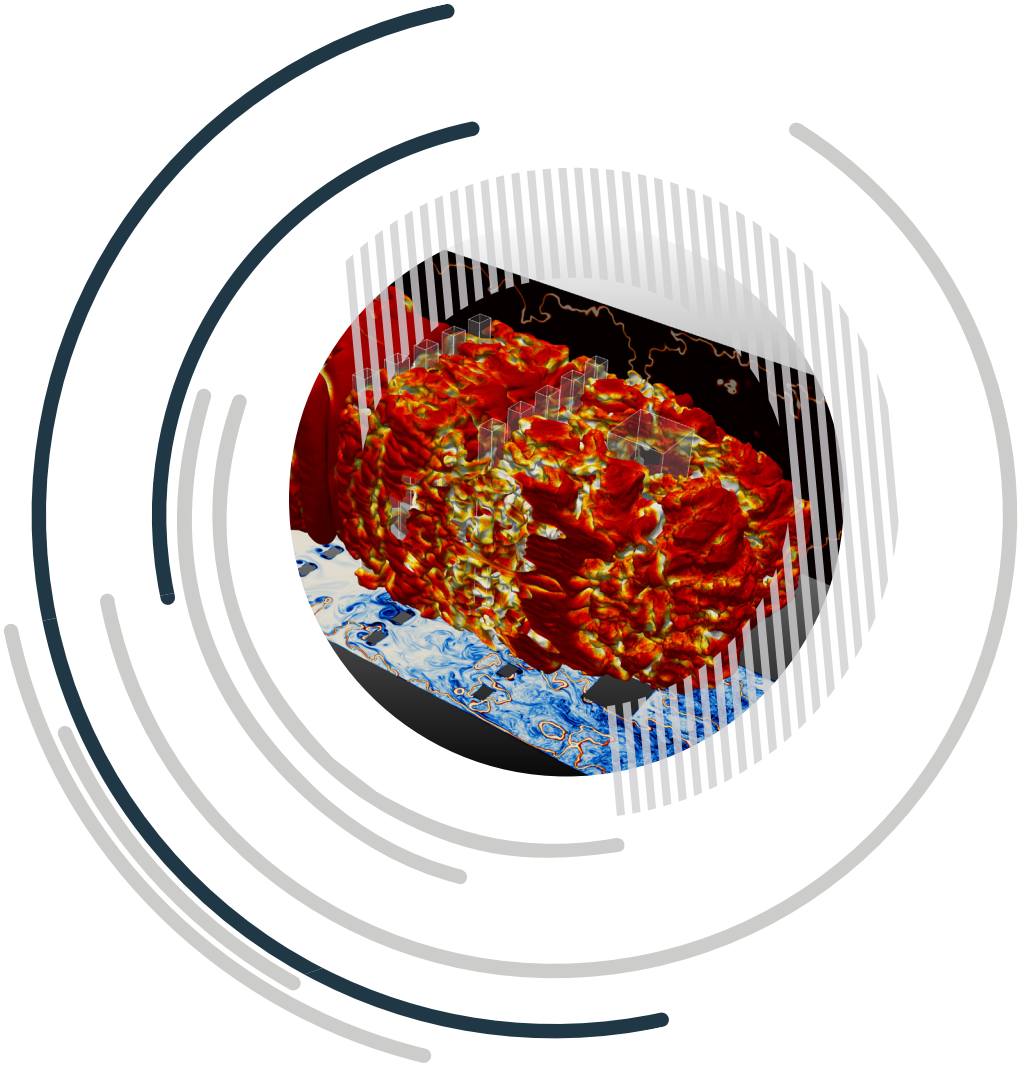
Note: Data is from calendar year 2014.

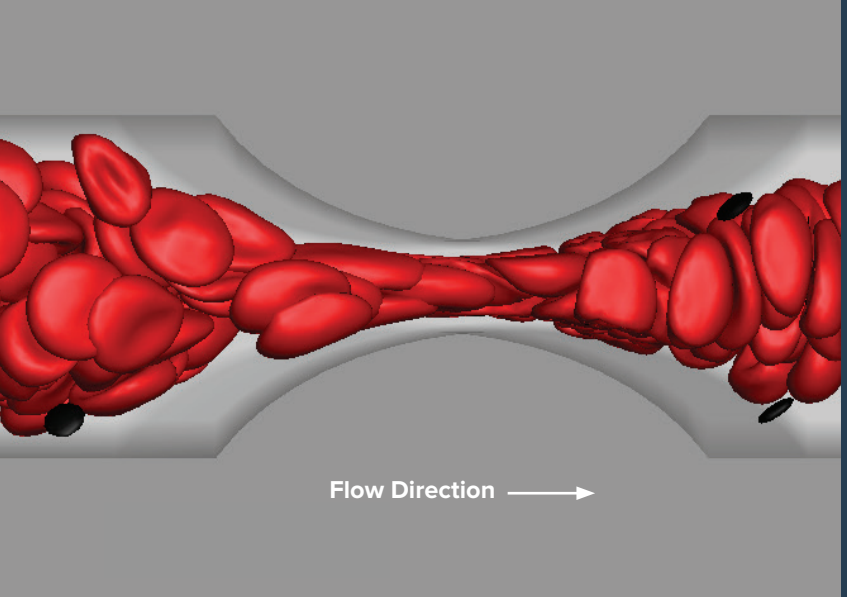


Cerebral aneurysms occur in up to 5 percent of the general population, leading to strokes for over 40,000 Americans each year. Rupture of a cerebral aneurysm can be a devastating event that kills or disables over 60 percent of afflicted patients. Currently, there exists no formal framework for the diagnosis of these aneurysms. Moreover, assessing the risk of a potential rupture is far from being fully understood. However, it is believed that factors such as location, geometry, blood flow patterns and resulting mechanical stresses within the aneurysm play a prominent role.

Image credit: Joseph A. Insley and Michael E. Papka, Argonne National Laboratory; George Em. Karniadakis, Paris Perdikaris, and Yue Yu, Brown University; Leopold Grinberg, IBM T. J. Watson Research Center and Brown University

SCIENCE HIGHLIGHTS





Biological Sciences

MULTISCALE SIMULATIONS of Human Pathologies

GEORGE KARNIADAKIS
Brown University
george_karniadakis@brown.edu
INCITE | 45 Million Core-Hours

RESEARCH CHALLENGE

Thoracic aortic aneurysm and dissection (TAAD) occurs when an aneurysm in the aorta expands and causes a tear in the artery wall. This condition is estimated to be responsible for around 30,000 deaths per year in the U.S. alone, but it 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 roles played by thrombi (blood clots) in aortic dissections.

APPROACH

Building on extensive computational expertise and past INCITE awards, researchers from Brown University have developed a flexible approach that integrates multiple computer codes to perform truly multiscale simulations of realistic biological systems. They are 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 also 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.

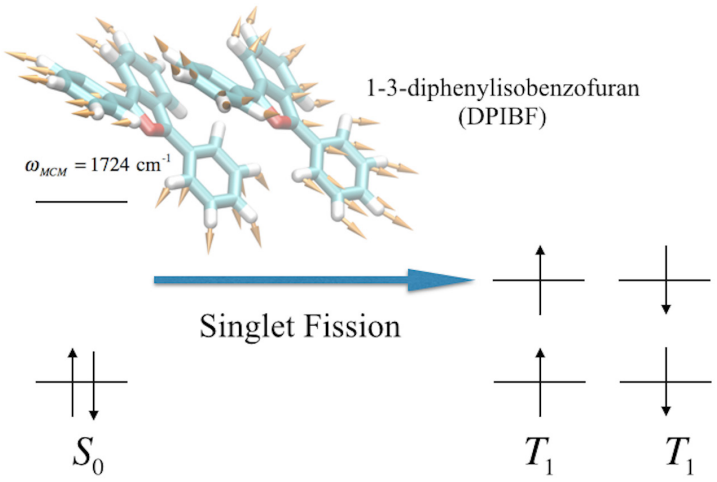
RESULTS

The researchers have studied platelet aggregation growth rates by simulating blood flow in a microvessel at different flow rates. The simulations predicted thrombi 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 thrombi 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.

Image caption: Snapshot of the whole-blood simulation in a micro-channel device with 75 percent degree stenosis. Image credit: George Em Karniadakis, Xuejin Li, and Zhen Li, Brown University



Chemistry

MOLECULAR MODELING of Singlet Fission for Solar Energy Conversion

HANNING CHEN
George Washington University
chenhanning@gwu.edu
Director's Discretionary | 6 Million Core-Hours

RESEARCH CHALLENGE

Singlet fission is a promising solution to long-standing roadblocks to more efficient solar energy conversion. The process converts two singlet molecules into two triplets upon the absorption of a single incident photon. This project investigates the molecular mechanism of this photo-induced spin separation process in a rich library of crystalline materials by a novel functional mode electron transfer theory.

APPROACH

Research efforts have focused on large-scale molecular dynamics calculations to ascertain a full spectrum of vibrational normal modes of the 1-3-diphenylisobenzofuran (DPIBF) thin film before the spin separation process is examined by hybrid quantum mechanics/molecular mechanics simulations. ALCF was integral in helping researchers skillfully run the open-source molecular simulation package CP2K at petascale on Mira, rendering a detailed picture of thermally driven spin transfer in molecular crystals.

Petascale simulations provide free-energy profiles along the reaction coordinate of singlet fission in addition to the projection of the associated reorganization energy onto a large number of vibrational normal modes.

RESULTS

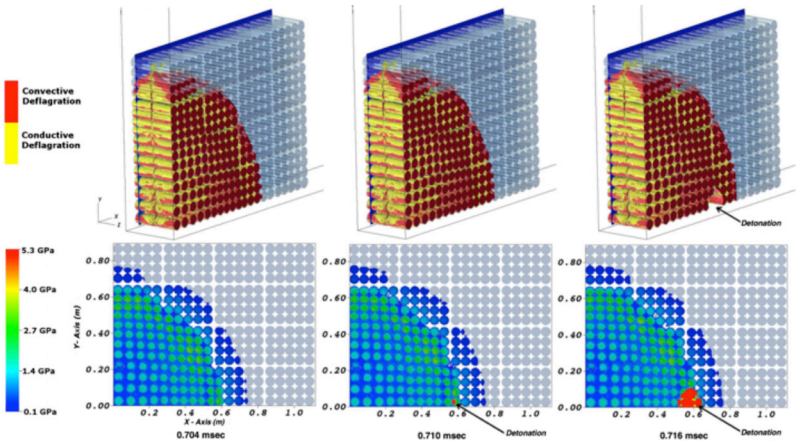
The researchers found that a specific vibrational mode of DPIBF is strongly correlated with the photo-induced spin separation, also suggesting a very strong vibronic coupling during singlet fission in DPIBF, due to the excessively large reorganization energy.

More importantly, the strong vibronic coupling in DPIBF thin film indicates the feasibility of improving singlet fission efficiency by modifying the vibrational density of states by temperature. For example, the pronounced anharmonicity of softened optical phonons at higher temperatures may result in a slower spin relaxation, responsible for the lower triplet quantum yield as observed by experiments.

IMPACT

The results of this research deepen an understanding of singlet fission at the electronic structure level of theory, such as the interplay between atomic displacements and electronic wave functions. Such a detailed comprehension will expedite the journey towards optimal solar energy conversion using environmentally friendly organic materials.

Image caption: Photo-induced spin polarization within a pair of DPIBF molecules. Image credit: Hanning Chen, George Washington University



Chemistry

SOLVING PETASCALE PUBLIC HEALTH AND SAFETY PROBLEMS Using Uintah

MARTIN BERZINS
University of Utah
mb@sci.utah.edu
INCITE | 200 Million Core-Hours

RESEARCH CHALLENGE

In 2005, a semi-truck hauling 35,000 pounds of explosives through the Spanish Fork Canyon in Utah crashed and caught fire, causing a dramatic explosion that left a 30-by-70-foot crater in the highway. Such accidents are extremely rare but can obviously have devastating results. A better understanding of exactly how such explosions occur is an important step to learning how to prevent them.

APPROACH

Researchers from the University of Utah used Mira to perform large-scale 3D simulations to study the physical mechanisms that led to the 2005 explosion, which was brought on by a process called deflagration-to-detonation transition (DDT). To achieve the high spatial and temporal resolution needed to carry out the multiscale, multiphysics simulations, the Utah researchers optimized their highly scalable Uintah Computational Framework to take advantage of Mira's petascale power. This involved leveraging the massively parallel capabilities of Uintah to develop a robust reaction model capable of simulating different modes of combustion at large scales.

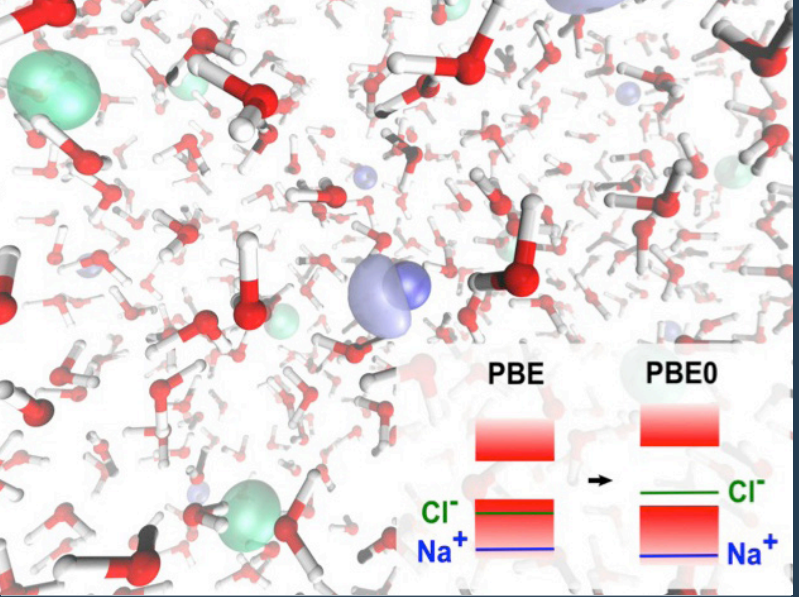
RESULTS

The team's simulations have yielded two possible mechanisms for DDT in large arrays of explosives. One hypothesis points to inertial confinement, a process in which damaged cylinders of explosives form a barrier that traps product gases, creating a pocket of high pressure that could initiate DDT. The other proposed mechanism involves a shock-to-detonation transition caused by the impact of explosive cylinders colliding in a high-pressure environment. More analysis is required before these theories can be confirmed or rejected. In addition to investigating why DDT occurred, the researchers examined how different packing densities and configurations could be used to prevent future explosions.

IMPACT

With a better understanding of the DDT process and the development of 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.

Image caption: The top figure shows the progression of deflagration through the explosive cylinders (light blue) transitioning to detonation (0.710 msec). The dark blue region shows the position of the 2D pressure slice illustrated in the bottom figure. Image credit: Jacqueline Beckvermit, Martin Berzins, Andrew Bezdjian, Todd Harman, Alan Humphrey, Qingyu Meng, and John Schmidt, University of Utah; Charles Wight, Weber State University



Chemistry

VIBRATIONAL AND OPTICAL SPECTROSCOPY of Electrolyte/Solid Interfaces

GIULIA GALLI
University of Chicago
gagalli@uchicago.edu

FRANCOIS GYGI
University of California, Davis
fgygi@ucdavis.edu

INCITE | 70 Million Core-Hours

RESEARCH CHALLENGE

Photoelectrochemical (PEC) energy conversion is a promising approach for producing hydrogen. The process uses solar energy to split water into hydrogen and oxygen gases. PEC cells have been suggested as one way to store solar energy in hydrogen for use as fuel. One of the key challenges to developing scalable, commercially viable PEC cells is to identify stable and efficient photoelectrode materials. A better understanding of PEC processes at the microscopic scale is needed so that these photoelectrodes can be developed.

APPROACH

For this INCITE project, researchers from the University of Chicago and the University of California, Davis, carried out large-scale simulations on Mira to model the physical and chemical processes occurring at the interface between solid photoelectrodes and electrolytes. 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. ALCF staff worked with the team to leverage parallel I/O libraries, port codes to Mira, and improve performance of Qbox and Quantum Expresso codes.

RESULTS

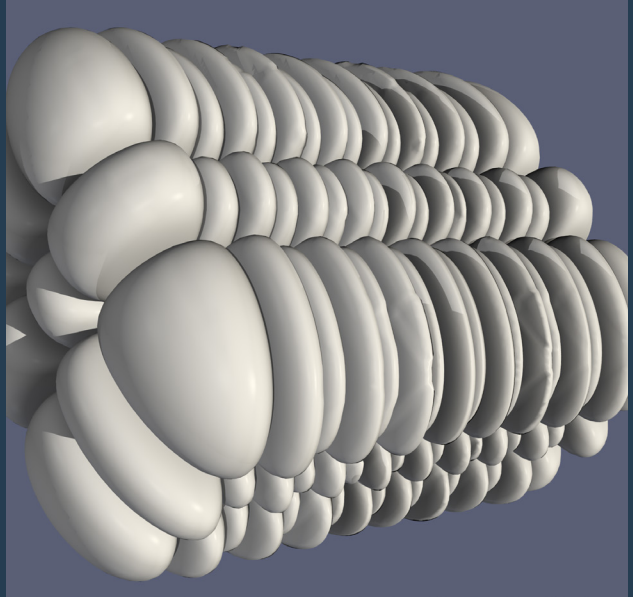
The use of hybrid functionals, combined with the massively parallel capabilities of Mira, allowed the researchers to calculate the electronic properties of electrolytes, a challenging task for *ab initio* simulations. This computational approach was applied to both sodium chloride and sulfuric acid in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

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 (an approximation used to calculate the self-energy of many-body systems), enabling GW calculations of unprecedented size for slabs containing solid-liquid interfaces.

IMPACT

This project provides knowledge and computational tools to interpret and inform ongoing experiments related to 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. The methodologies and results stemming from this work are also relevant to other energy-related research efforts, including electrical energy storage and solar cells.

Image caption: Snapshot of a 1 mol/L solution of NaCl obtained from an *ab initio* molecular dynamics simulation with a hybrid (PBE0) functional. Image credit: Alex Gaiduk, University of Chicago



Computer Science

DYNAMIC AND ADAPTIVE PARALLEL PROGRAMMING for Exascale Research

ROBERT HARRISON
Brookhaven National Laboratory
rjharrison@gmail.com
INCITE | 20 Million Core-Hours

RESEARCH CHALLENGE

The path from petascale to exascale computing poses many challenges for the developers of hardware architectures, system software, and applications. This project continues 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.

APPROACH

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

RESULTS

Researchers have used Mira to develop high-performance kernels using code generation/transformation with polyhedral analysis and autotuning. They have also tested Intel® Threading Building Blocks with the aim of replacing MADNESS's 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.

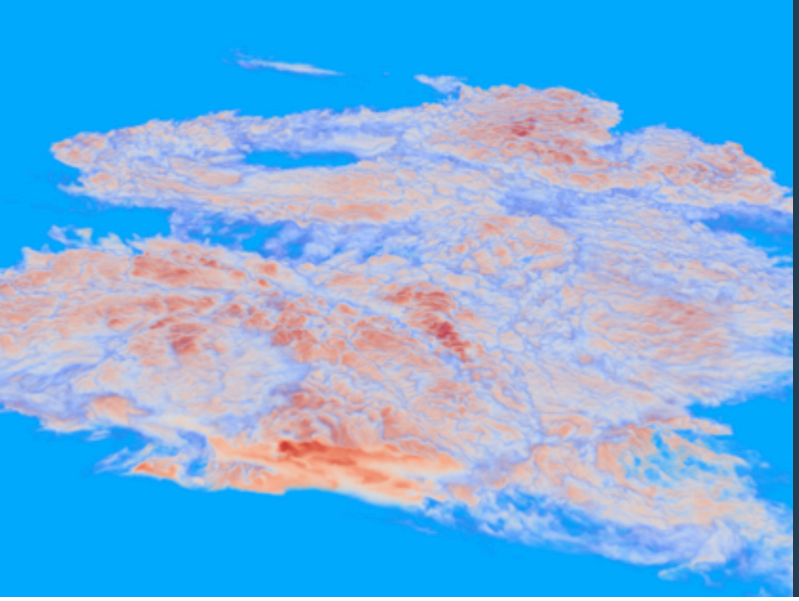
For the DFT code, the team has implemented pseudopotentials, which reduce the number of electrons that are explicitly treated and therefore decrease the cost of molecular simulations. Work is ongoing to integrate a newly implemented approach to calculating inner products in MADNESS.

The 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 DFT 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 supports the very active community developing and employing high-performance and high-productivity parallel programming paradigms in anticipation of the transition from petascale to exascale computing. These paradigms provide a natural and fully compatible extension of MPI (message passing interface) 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.

Image caption: 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



Earth Science

EVALUATION OF MESOSCALE ATMOSPHERIC MODEL for Contrail Cirrus Simulations

ROBERTO PAOLI
CERFACS
paoli@cerfacs.fr
INCITE | 25 Million Core-Hours

RESEARCH CHALLENGE

Contrails, the visible white lines in the sky left behind an airplane, are ice clouds made by 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 more contrail cirrus is of increasing concern for scientists and policymakers. This research utilizes ALCF computing resources to fine-tune numerical models that will provide a more accurate understanding of contrail cirrus impact on global climate.

APPROACH

The team used Meso-NH, a non-hydrostatic mesoscale atmospheric simulation model, to analyze the evolution of the contrail cirrus up to one hour after emission. They simulated three cases of contrails utilizing background turbulence generated during earlier stages of the project.

RESULTS

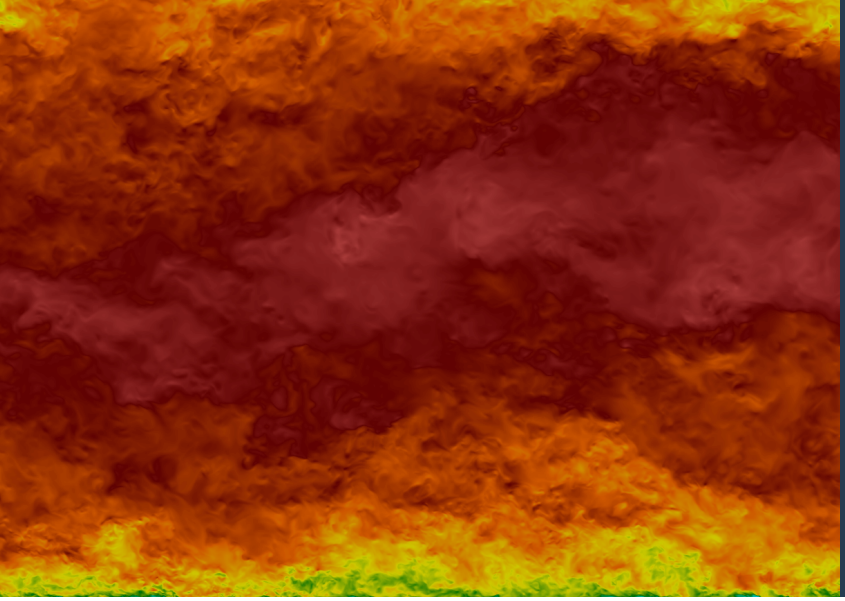
An important result of the study is that radiative transfer—the absorption, emission, and scattering of electromagnetic radiation—is the key mechanism controlling the global ice characteristics and the vertical extension of the contrail, and is predominant on the atmospheric turbulence one hour after the contrail has formed. This effect is magnified during the day by direct heating, mostly at the top of the contrail in the visible band of the spectrum that adds to the heating at the bottom in the infrared band from the Earth's surface.

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.

IMPACT

By understanding and characterizing the physical mechanisms that control the formation of contrail cirrus, this INCITE research is leading to more complete and effective high-resolution atmospheric models for the development of parameterizations of aircraft perturbations in next-generation global and climate models.

Image caption: 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 of 1 mg/kg (blue) to 25 mg/kg (red). Atmospheric turbulence and radiative transfer modules are activated (day conditions). Image credit: Roberto Paoli and Odile Thouron, CERFACS



Engineering

DIRECT NUMERICAL SIMULATIONS of High Reynolds Number Turbulent Channel Flow

ROBERT MOSER
University of Texas at Austin
rmoser@ices.utexas.edu
INCITE | 175 Million Core-Hours

RESEARCH CHALLENGE

A substantial amount of the energy consumed by a moving vehicle or boat is due to the drag and dissipation of energy caused by turbulence as it moves through air or water. The same forces are at work as air or liquid moves through ducts or pipes. A large reference dataset describing the behavior of turbulence is needed to better understand and model this phenomenon.

APPROACH

Researchers from the University of Texas at Austin conducted the largest-ever direct numerical simulation (DNS) of this fluid dynamics problem—simulations at a Reynolds number (a dimensionless ratio of inertial forces to viscous force) of 5200 on a 15360 x 1536 x 11520 mesh. Of particular interest to the research team was the overlap region, where viscous near-wall turbulence interacts with outer-layer turbulences. Previous simulations did not allow for a high enough Reynolds number to obtain the scale separation needed to understand the complexity of this turbulent interaction. Due to the substantial power of Mira, the researchers were able to simulate a DNS with high enough Reynolds number to generate sufficient scale separation. Collaboration with ALCF staff helped improve the management of cache and execution threads, doubling code performance. They also achieved near-perfect OpenMP scalability (99 percent) by minimizing the inter-memory access between OpenMP threads.

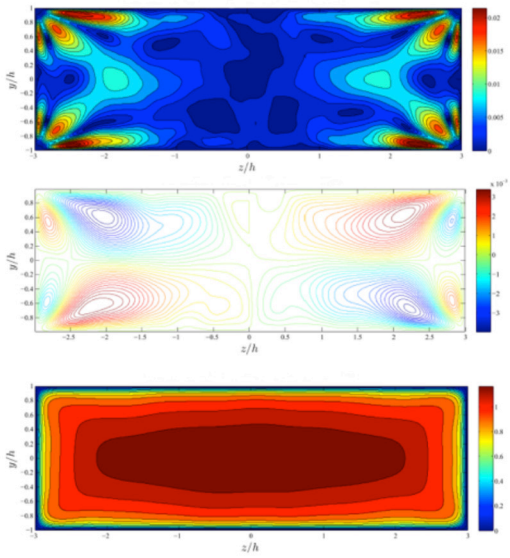
RESULTS

These simulations generated a new reference dataset that will remain useful for turbulence research for years to come. The channel flow data is now available for the public to use for calibrating their turbulence models, developing new turbulence models, and validating existing ones. The data is available online at http://turbulence.ices.utexas.edu/.

IMPACT

The models resulting from this project will allow faster, more effective studies of turbulence, such as air-flow over vehicles, and could lead to improved vehicle surfaces and reduced-drag piping and ducts. Data from the project is publicly available so it can be used by other researchers in their turbulence models and design projects.

Image caption: This visualization depicts the instantaneous streamwise velocity component over a section of the simulated channel. Image credit: Nicholas Malaya, University of Texas at Austin



Engineering

DOES A TURBULENT DUCT FLOW Ever Become Two-Dimensional?

HASSAN NAGIB
Illinois Institute of Technology
nagib@iit.edu
ALCC | 11 Million Core-Hours

RESEARCH CHALLENGE

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. A deeper understanding of flow physics in rectangular ducts is needed to enable the discovery of ways to reduce drag and friction, thereby reducing global energy consumption.

APPROACH

Traditional computational studies of turbulent flow within a duct have always assumed that the duct can be treated as infinitely wide (2D) if the duct is wide enough. However, recent experiments at the Illinois Institute of Technology (IIT) have shown that this 2D assumption is not representative of the physical flow for many realistic flow regimes. To better understand the experimental results, IIT researchers carried out simulations on ALCF supercomputers with Nek5000, a highly scalable computational fluid dynamics code. The simulations allowed them to study the behavior of turbulent flow through rectangular ducts for an increased number of aspect ratios and more realistic Reynolds numbers.

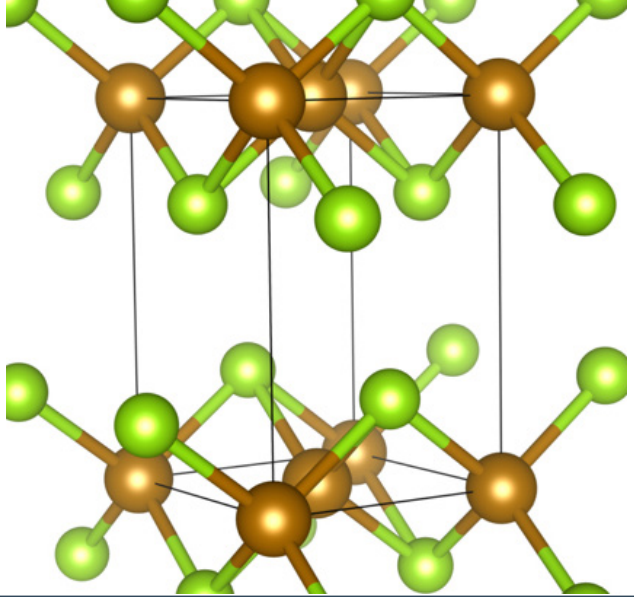
RESULTS

Several duct aspect ratios (ratio of width/length) were studied using computational fluid dynamics. At higher aspect ratios (ranging from 12.8 to 48), the calculated skin friction decreases as the aspect ratio increases up to 24, where it then appears to reach an asymptotic value—this agrees well with experimental data. However, when increasing the aspect ratio from 1 to 3, the friction actually increases rather than decreases. It was determined that the increased friction results from a complex relationship between the side-wall boundary layer thickness and secondary motions in the flow. These secondary motions significantly impact the overall flow physics but have not been reported 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 Reynolds number and aspect ratio. Understanding these 3D effects through computation leads to improved computational models and better fundamental understanding of the flow physics.

IMPACT

The simulations from this project have shed light on the existence of important fluid flow physics that have been postulated but are 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 friction in a variety of applications.

Image caption: In-plane velocity, streamlines and streamwise velocity of the aspect ratio 3 case. Image credit: Hassan Nagib, Illinois Institute of Technology



Materials Science

CORRELATED ELECTRONS in Photoactive and Superconducting Materials

LUCAS K. WAGNER
University of Illinois at Urbana-Champaign
lkwagner@illinois.edu
INCITE | 60 Million Core-Hours

RESEARCH CHALLENGE

Although the existence of high-temperature superconductors (materials that conduct electricity at temperatures higher than 30 degrees Kelvin) has been known for years, the microscopic origin of their properties has remained elusive. The behavior of these materials is dependent on the interaction of their electrons. Since the equations governing quantum particles are computationally complex, predicting the properties of materials is a difficult task that is not possible with traditional methods like density functional theory (DFT). Another approach is needed to understand how materials become high-temperature superconductors.

APPROACH

For this INCITE project, researchers at the University of Illinois at Urbana-Champaign (UIUC) used quantum Monte Carlo (QMC) methods to advance the understanding of high-temperature superconductivity by explicitly simulating the interactions between electrons. The advent of massively parallel supercomputers like Mira has brought the QMC method to the forefront and permitted calculations that were previously only accessible by computationally cheaper and less accurate methods such as DFT. The UIUC team used their QWALK code to perform diffusion Monte Carlo calculations on iron selenide (FeSe), a known high-temperature superconductor.

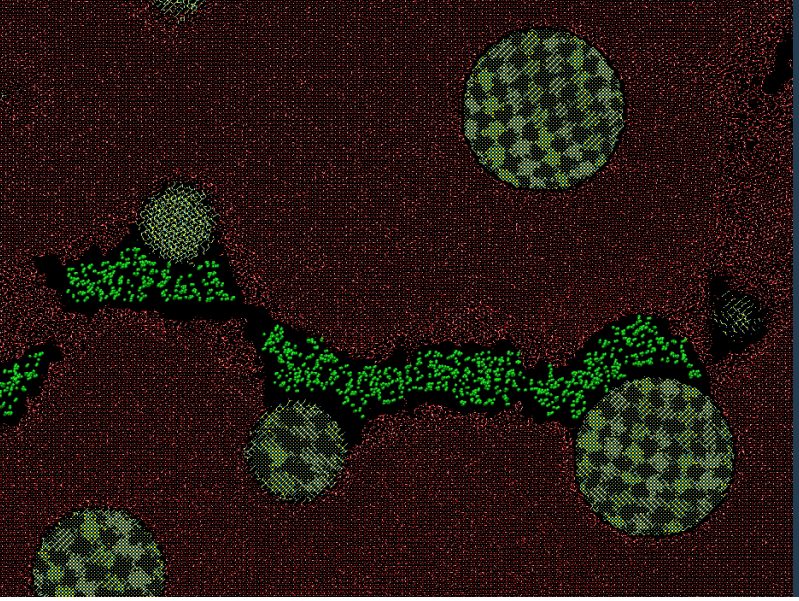
RESULTS

In experiments, FeSe starts with a low critical temperature and becomes superconducting as pressure is applied; with more pressure, the superconductivity vanishes. To better understand how superconductivity emerges in FeSe, the UIUC researchers aimed to shed light on FeSe's electron-spin interaction, which increases under pressure. This involved carrying out QMC calculations on Mira to study the magnetic state of FeSe at varying pressures. Their calculations added to the existing body of evidence supporting the notion that high-temperature superconductivity is magnetic in origin.

IMPACT

The team's studies of FeSe represent the first application of this level of QMC to these materials, providing evidence for the magnetic origin of superconductivity. Findings from this effort will also help improve the fundamental understanding of electronic matter, which will aid scientists in the development of new materials and better control of existing materials, thus paving the way for new devices to meet our nation's energy challenges.

Image caption: Iron selenide is a known high-temperature superconductor. Image credit: Lucas K. Wagner, University of Illinois at Urbana-Champaign



Materials Science

PETASCALE SIMULATIONS of Self-Healing Nanomaterials

RAJIV KALIA
University of Southern California
rkalia@usc.edu
INCITE | 200 Million Core-Hours

RESEARCH CHALLENGE

Self-healing nanomaterials are capable of sensing and repairing damage, such as cracks, in devices operating in harsh conditions. With the ability to enhance reliability and reduce maintenance costs, these materials show great promise for use in energy technologies, such as high-temperature turbines. To advance the viability of these materials, researchers need a better understanding of the atomistic mechanisms underlying the remarkable self-healing capabilities.

APPROACH

Researchers from the University of Southern California (USC) are using ALCF resources to carry out quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and mesoscale simulations of two types of self-healing 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 USC 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.

RESULTS

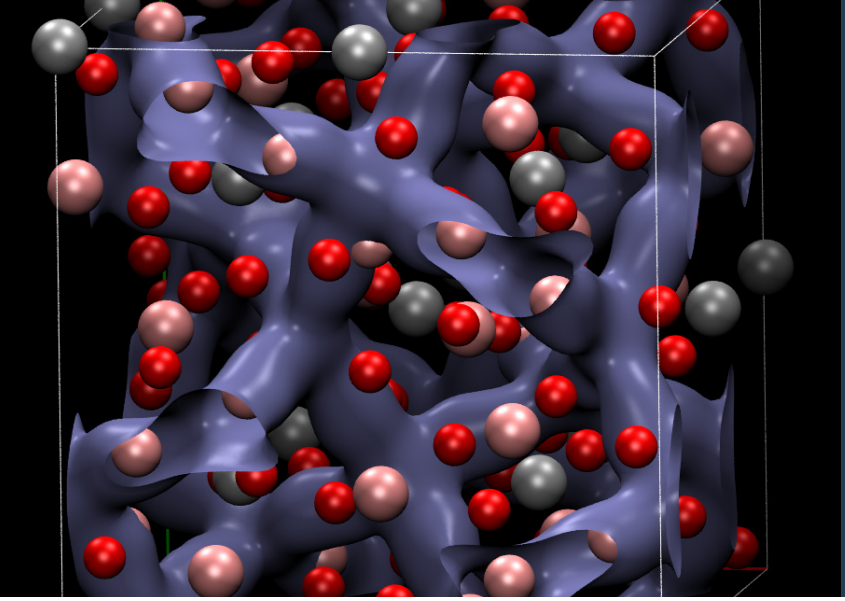
Their efforts have resulted in excellent weak-scaling and strong-scaling parallel efficiencies (0.984 and 0.803 on the full machine, respectively), improved time to solution (60 times faster than previous state-of-the-art calculations), and improved performance (from 30 percent to 50.5 percent of Mira's theoretical peak, or 5.1 petaflops). The team successfully used this code in a previous INCITE project to study hydrogen production from aluminum-water reactions. Those massive QMD simulations are now 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.

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.

Image caption: 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



Materials Science

PREDICTIVE MATERIALS MODELING for Li-Air Battery Systems

LARRY CURTISS
Argonne National Laboratory
curtiss@anl.gov
INCITE | 100 Million Core-Hours

RESEARCH CHALLENGE

With the potential to store up to 10 times the energy of a lithium-ion (Li-ion) battery of the same weight, lithium-air (Li-air) batteries are viewed as a possible game changer for electric vehicles. But realizing their enormous potential 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.

APPROACH

Scientists from Argonne National Laboratory and IBM Research are using Mira to conduct *ab initio* density functional theory (DFT) simulations to better understand the physical and chemical mechanisms of Li-air batteries. Their objective is to accelerate efforts to identify novel materials for electrolytes.

RESULTS

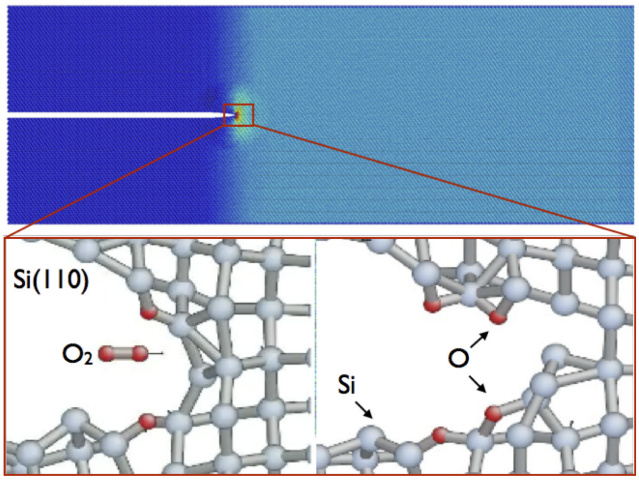
In a recent study, IBM researchers focused on the zirconium-containing, garnet-like lithium-lanthanum-oxide, known as LLZO, a promising material for solid-state electrolytes. Experimental work has determined that the cubic phase of LLZO is much better at conducting Li-ions than its tetragonal phase, 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 simulated time scales in nanoseconds rather than picoseconds. They were able to achieve this factor-of-a-thousand improvement by using metadynamics (a method for accelerating rare events, such as mapping the conductivity of a material regardless of its complexity) into their DFT simulations. 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.

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 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.

Image caption: 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



Materials Science

SiO2 FRACTURE: Chemo-mechanics with a Machine Learning Hybrid QM/MM Scheme

JAMES KERMODE
University of Warwick
j.r.kermode@warwick.ac.uk
INCITE | 125 Million Core-Hours

RESEARCH CHALLENGE

The fracture and cracking of brittle materials belongs to the class of chemo-mechanical phenomena for which there is not yet an in-depth understanding, despite the obvious relevance for saving energy in widespread industrial applications, such as mining. Atomistic simulations offer an attractive avenue by which to develop comprehensive predictive modeling and simulation tools. Unfortunately, these phenomena occur at such significant length-scales that quantum mechanics alone cannot be used to model all atoms equally.

APPROACH

Researchers have been using Mira to model several hypothesized silicon dioxide (SiO_2) crack propagation processes. Access to Mira enabled a ten-fold increase in sampling time, thereby strengthening significantly the numerical evidence for the findings made.

The team applied a hybrid multiscale simulation program that combines various levels of theories to help describe the fracturing of silicon and SiO_2. This quantum mechanical/molecular mechanical (QM/MM) scheme combines less expensive and less accurate force-field potentials for most atoms with more expensive and more accurate quantum mechanics-derived potentials for few reactive atoms near to crack tips. This allows multiple spatial scales to be treated in a consistent fashion, while long time scales can be accounted for through interpolation of atomic forces using statistical methods, such as Machine Learning.

As the INCITE project develops, the QM/MM approach will be coupled with a Machine Learning method called "Learn on the Fly," which is of particular interest since it enables the systematic study of large systems with QM precision, for the first time.

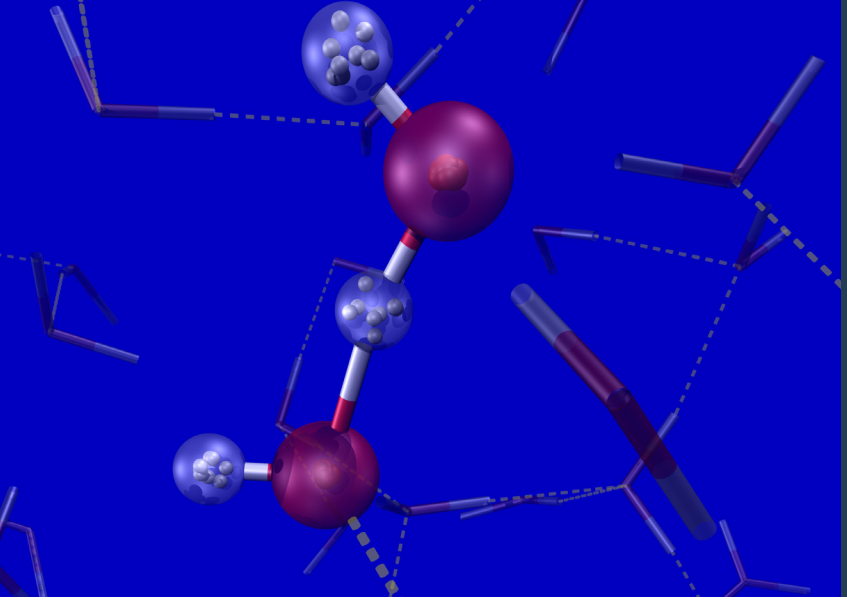
RESULTS

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. Work is ongoing to extend these findings to the technologically relevant case of SiO_2, in both its crystalline (rock) and amorphous (glass) forms, and in wet and dry environments.

IMPACT

Understanding of crack propagation has been deepened, and the role of oxygen in SiO_2 cracking has been elucidated. Simulation results have also been confirmed by experiment. New algorithms have been implemented and deployed successfully for high-performance computing resources.

Image caption: 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, University of Warwick



Physics

AB INITIO QUANTUM Liquid Water and Aqueous Ionic Solutions

ROBERT A. DISTASIO JR.
Princeton University
distasio@princeton.edu
ALCC | 250 Million Core-Hours

RESEARCH CHALLENGE

A highly accurate and detailed understanding of the microscopic structure of liquid water is critical to a number of fields, ranging from energy storage to biochemistry and environmental sciences. *Ab initio* molecular dynamics (AIMD) based on density functional theory is the most accurate and widely used computational methodology for modeling condensed phase systems, but this approach has severe limitations when applied to liquid water.

APPROACH

For this ALCC project, researchers from Princeton University combined novel theoretical and algorithmic developments to create an innovative approach that has enabled highly accurate atomistic simulations of liquid water on Mira. They also applied this approach to aqueous ionic solutions that are relevant to the design of clean energy materials, such as electrolytes for aqueous-ion batteries. ALCF staff collaborated with the researchers to develop a new multi-threaded version of the 3D Poisson solver used in these calculations.

RESULTS

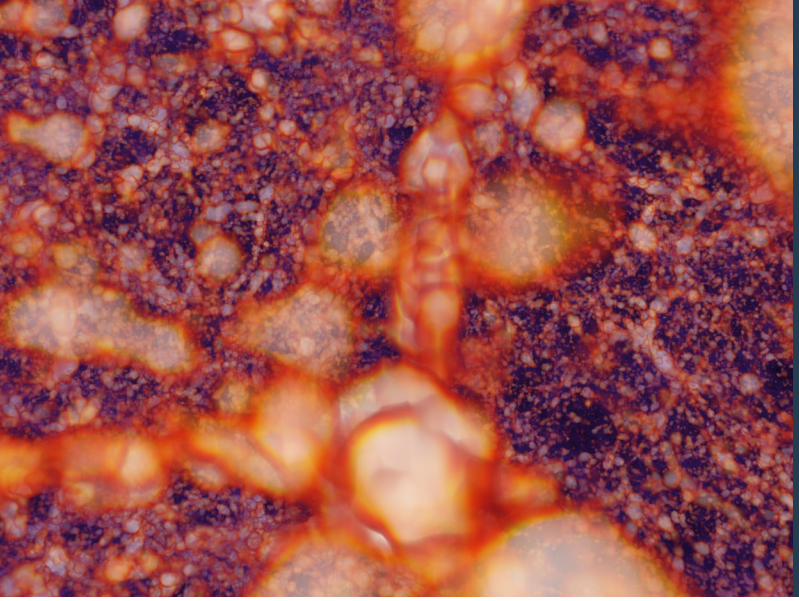
The researchers have completed several production-level path integral (PI)-AIMD simulations of liquid water at the PBE, PBE+vdW, and PBE0+vdW levels of theory. These simulations allowed them to accurately capture the main experimental isotope effects in the oxygen-oxygen, oxygen-hydrogen, and hydrogen-hydrogen 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 and hydroxide ionic solutions (models of acidic and basic conditions, respectively). The proton transfer rates from these simulations showed excellent agreement with experimental data.

Their work has also determined the importance of exact exchange and non-local van der Waals interactions in predicting the anomalous density ordering between crystalline ice and liquid water—an unusual property of water that has posed a substantial challenge for theory to date.

IMPACT

These simulations are providing detailed knowledge of the microscopic structure of liquid water and aqueous ionic solutions with unprecedented accuracy. The results will be stored in a public database and will serve as a valuable resource for other theoretical and experimental work. This data will help advance clean energy applications, such as the design of aqueous-ion batteries.

Image caption: 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



Physics

COSMOLOGICAL SIMULATIONS for Large-Sky Surveys

SALMAN HABIB
Argonne National Laboratory
habib@anl.gov
INCITE | 200 Million Core-Hours
(ALCF: 100 Million; OLCF: 100 Million)

RESEARCH CHALLENGE

Modern precision cosmology provides the key underpinnings for most investigations of the yet-unidentified fundamental constituents of our universe, dark matter and dark energy. Large-scale simulations of structure formation in the universe are essential for interpreting data from wide and deep cosmological surveys, as well as for optimizing survey design. Extracting fundamental physics knowledge from the statistics of the observed spatial distribution of celestial objects (e.g., galaxies, quasars, galaxy clusters) requires a comparison to predictions from a large number of different simulations.

APPROACH

Project simulations are carried out with the extreme-scale Hardware/Hybrid-Accelerated Cosmology Code (HACC), which solves for the gravitation-dominated evolution of matter in the universe using an N-body approach. HACC has been architected for portability across supercomputing architectures, and extensively optimized for Mira.

RESULTS

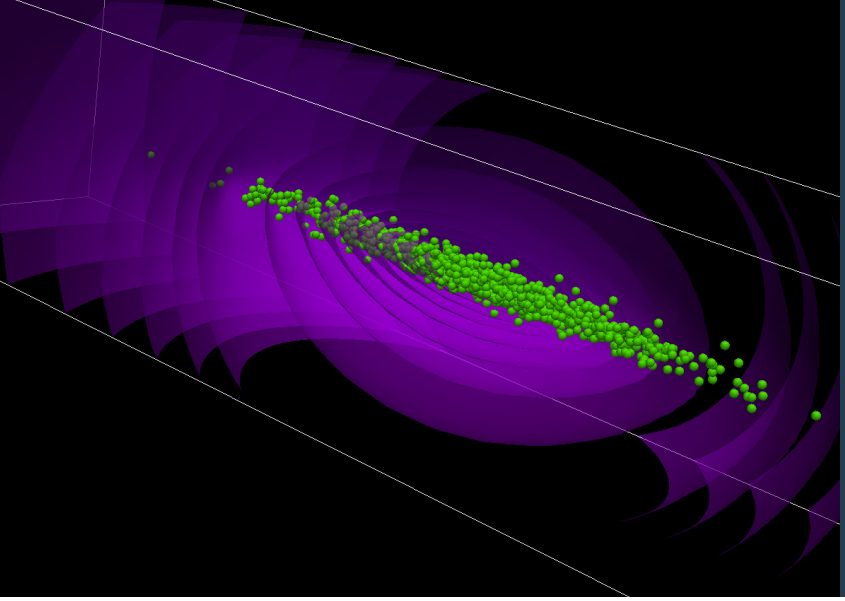
The Outer Rim simulation, the largest high-resolution cosmological simulation carried out to date, modeled the evolution of over one-trillion tracer particles, on 32 racks of Mira. Covering a large portion of the observed universe, it resolves the dark matter-dominated clumps, or halos, that host galaxies and quasars. The simulation created 100 full time snapshots, in effect comprising a movie of the modeled universe, allowing researchers to extract details of the evolution of cosmic structure and to use this information to discover how different types of galaxies reside in different halos.

Halo property data extracted from five simulations was used to investigate the deviation of the halo mass function (number of halos as a function of mass) from a 'universal' form. These early results confirm the effectiveness of the 100-simulation suite that is planned for this project.

IMPACT

The Outer Rim simulation is being analyzed to generate object catalogs for several different upcoming cosmological surveys, and has been used to create a synthetic catalog for the Dark Energy Spectroscopic Instrument (DESI) project. Cluster-scale halos from the simulation have been used to create strong lensing maps to study clusters observed by the Hubble Space Telescope and by large ground-based telescopes.

Image caption: This image shows a large simulation of the distribution of matter in the universe, the so-called cosmic web, which evolved under the influence of dark energy. The simulation was run with 1.1 trillion particles using HACC, a simulation framework developed with the challenges of future supercomputing architectures in mind. Image credit: Hal Finkel, Nicholas Frontiere, Salman Habib, Katrin Heitmann, Mark Hereld, Joseph Insley, Kalyan Kumaran, Vitali Morozov, Michael E. Papka, Tom Peterka, Adrian Pope, and Tim Williams, Argonne National Laboratory; Zarija Lukic, Lawrence Berkeley National Laboratory; David Daniel and Patricia Fasel, Los Alamos National Laboratory



Physics

INTENSITY-DEPENDENT DYNAMICS in Fermilab and CERN Accelerators

JAMES AMUNDSON
Fermilab
amundson@fnal.gov
INCITE | 50 Million Core-Hours

RESEARCH CHALLENGE

Particle accelerators are an enabling technology for both basic research and the applied sciences. The future of high energy physics requires running today's accelerators at higher intensities than ever before. To accurately understand intensity-dependent effects in their accelerators' complexes, researchers at both Fermilab and CERN are relying on advanced detailed numerical modeling.

APPROACH

Researchers from Fermilab are using ALCF resources to perform complex accelerator simulations aimed at reducing the risks and costs involved in developing the world's highest intensity particle beams. ALCF assisted in porting Synergia, a hybrid C++-Python code to the Blue Gene/Q platform and finding optimizations specific to Mira's architecture.

The Fermilab Recycler and Main Injector form the final high-energy stage of the Fermilab accelerator complex. During each acceleration cycle, the Recycler receives protons in six batches from the booster. Through a radio frequency manipulation procedure known as slip-stacking, the batches are combined to increase the instantaneous intensity. The protons are then transferred to the Main Injector where they are accelerated from 8 GeV to 120 GeV.

RESULTS

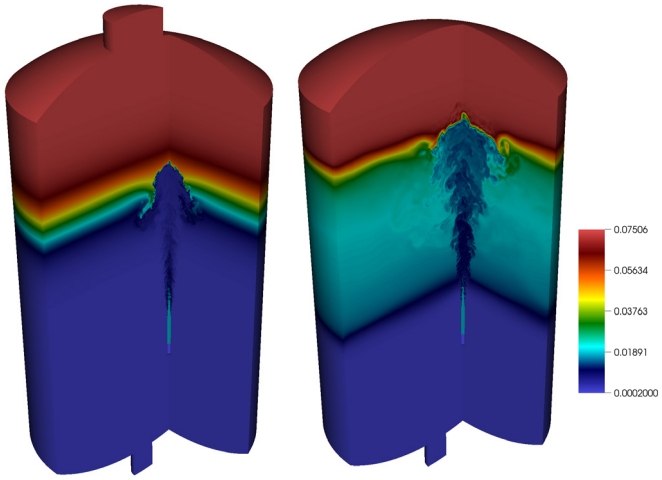
Simulations of the Booster have been focused on understanding further details of instability generation caused by the wakefield mechanism, in which a charged particle traveling through a conducting pipe generates fields that affect trailing particles. Researchers have succeeded in reproducing theoretically predicted strong space charge modes in Synergia under simplified conditions.

The Fermilab Recycler is being used to slip-stack at much higher intensities than has been performed previously. Current slip-stacking simulations of the Recycler aim to understand whether this energy difference combined with the space charge effects of higher intensity beams will result in increased particle losses.

IMPACT

These simulations will advance an understanding of the dynamics of intense particle beams, which will be used to create neutrino sources for the Long Baseline Neutrino Experiment at Fermilab and for the upgrade to the Large Hadron Collider at CERN. Beyond the realm of particle physics, this accelerator technology potentially could impact basic energy applications, such as the transmutation of nuclear waste.

Image caption: Synergia simulation of a bunched beam including particles (green) and self-fields (purple). Image credit: James Amundson, Fermilab



Physics

THERMAL HYDRAULIC MODELING: Cross-Verification, Validation, and Co-Design

PAUL FISCHER
Argonne National Laboratory
fischer@msc.anl.gov
INCITE | 60 Million Core-Hours

RESEARCH CHALLENGE

The ability to control convection and mixing of buoyant flows can play an important role in either the safety of or significant damage to nuclear containment facilities. The Organization for Economic Cooperation and Development's Nuclear Energy Agency chose this project as a PANDA experiment for a 2014 benchmark exercise, wherein predictive capabilities of computational fluid dynamics tools are tested for multispecies convection under a notorious transition regime from turbulent to laminar flow and from forced to natural convection. Accurate prediction of these phenomena will increase understanding of reactor behavior during accidents and help design safer and more efficient reactors for a carbon-free energy option.

APPROACH

Designed to study buoyancy, convection, and mixing flows, the PANDA experiment facility is a multi-compartment, large-scale thermal-hydraulics test rig located at the Paul Scherrer Institute in Switzerland. Initially, the experiment vessel contains a well-defined gas mixture of helium/air at the top, and air below with measured stratification.

A jet of air and buoyant helium is injected into the vessel which eventually erodes the initial stratification layer, posing significant challenges for accurate prediction of flow evolution. The spectral element code Nek5000 was used to conduct a series of numerical experiments to optimize computational cost and accuracy in this type of flow prediction.

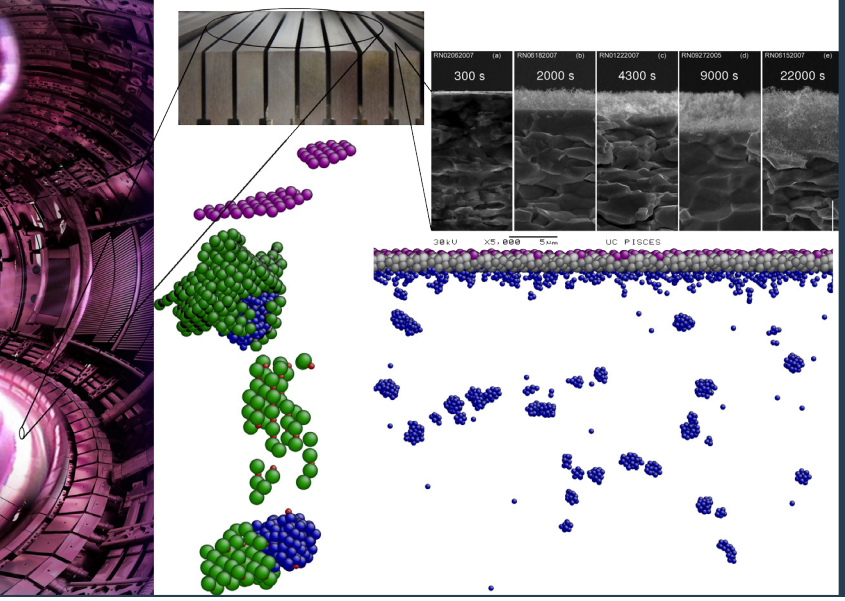
RESULTS

Insights were made into developing the best methods for simulating this difficult flow regime using Nek5000, including discovery of the optimal meshing, and changing the boundary conditions at the inlet. Varying approximations for modeling buoyancy and diffusion effects were tested to see the effect on the flow.

IMPACT

The Nek5000 code has now been studied under flow regimes previously not validated, which are important for nuclear reactor containment accident scenarios. Important insights were gained which will optimize computational cost and accuracy in this type of flow prediction. Eventually the results will be compared with the experimental benchmark data to validate Nek5000 in these conditions.

Image caption: 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



Physics

UNDERSTANDING HELIUM PLASMA MEDIATED TUNGSTEN SURFACE RESPONSE that Controls Plasma Facing Component Performance and Lifetime

BRIAN WIRTH
University of Tennessee, Knoxville
bdwirth@utk.edu
ALCC | 7.5 Million Core-Hours

RESEARCH CHALLENGE

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 the employment of 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, responsible for the removal of fusion reaction by-products.

APPROACH

Researchers utilized 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. Simulations have focused on implanting helium gas atoms below specific tungsten surfaces.

RESULTS

Recent scientific results have helped determine 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 a marked difference in the helium retained between different orientations/layers of surfaces, suggesting that a mechanism exists which prevents helium from leaving specific tungsten surfaces and not others, and that this mechanism is quite strong.

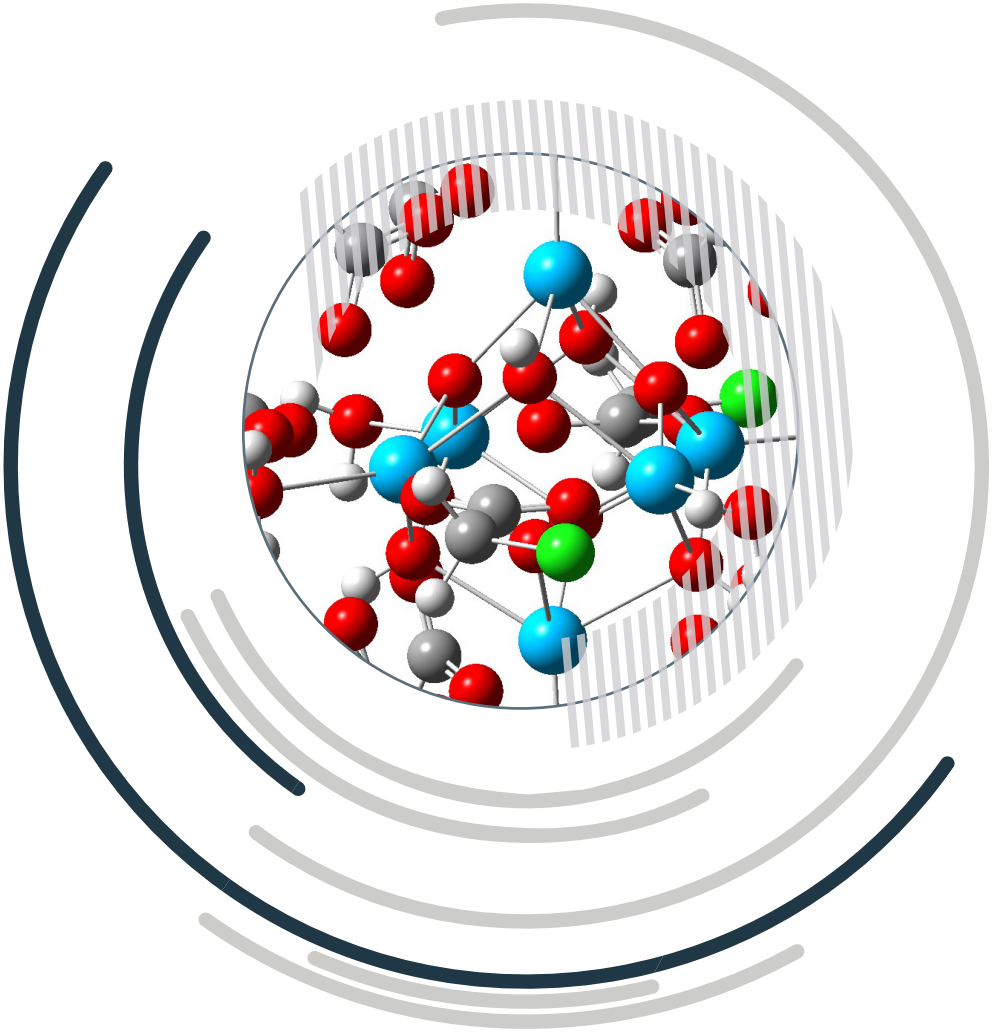
MD simulations have shown that surface damage can occur at the size of just a single helium atom, when helium is below a specific tungsten surface. This results in a very large concentration of helium atoms in substitutional tungsten positions. The presence of this helium layer may substantially influence the sputtering and erosion behavior of tungsten.

IMPACT

The results of this work may indicate that specific tungsten surface orientations are preferable for exposed surfaces of plasma-facing components. This understanding would lead to predictive modeling capabilities for materials design of the ITER divertor, allowing it to endure the incredibly extreme conditions of a fusion power plant.

Image caption: 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

2014 ALCF **PUBLICATIONS**



2014 ALCF **PUBLICATIONS**

Researchers who use ALCF resources are major contributors to numerous publications that document their breakthrough science and engineering. The refereed journal articles and conference proceedings represent research ventures undertaken at the ALCF through programs supported by the U.S. Department of Energy and Argonne National Laboratory.

The publications are listed in descending order of their publication dates. An asterisk after a name indicates an Argonne author. ALCF publications are listed online at http://www.alcf.anl.gov/publications.

Faney, T. and B. D. Wirth. "Spatially Dependent Cluster Dynamics Modeling of Microstructure Evolution in Low Energy Helium Irradiated Tungsten." *Modelling and Simulation in Materials Science and Engineering*, December 2014, vol. 22, no. 065010.

Horelik, N., A Siegel,* B. Forget, and K. Smith. "Monte Carlo Domain Decomposition for Robust Nuclear Reactor Analysis." *Parallel Computing*, December 2014, vol. 40, no. 10, 646-660.

Perdikaris, P., L. Grinberg, and G. E. Karniadakis. "An Effective Fractal-Tree Closure Model for Simulating Blood Flow in Large Arterial Networks." *Annals of Biomedical Engineering*, December 2014.

Roberts, N. V.* "Camellia: A Software Framework for Discontinuous Petrov-Galerkin Methods." *Computers & Mathematics with Applications*, December 2014, vol. 68, no. 11, 1581-1604.

Sharifzadeh, S., C. Y. Wong, H. Wu, B. L. Cotts, L. Kronik, N. S. Ginsberg, and J. B. Neaton. "Relating the Physical Structure and Optoelectronic Function of Crystalline TIPS-Pentacene." *Advanced Functional Materials*, December 2014.

Sillero, J. A., J. Jiménez, R. D. Moser. "Two-Point Statistics for Turbulent Boundary Layers and Channels at Reynolds Numbers Up to $\delta+ \approx 2000$." *Physics of Fluids*, December 2014, vol. 26, no. 10.

Solomonik, E., D. Matthews, J. R. Hammond, J. F. Stanton, and J. Demmela. "A Massively Parallel Tensor Contraction Framework for Coupled-Cluster Computations." *Journal of Parallel and Distributed Computing*, December 2014, vol. 74, no. 12, 3176-3190.

Vázquez–Mayagoitia, A.,* W. S. Thornton, J. R. Hammond,* and R. J. Harrison. "Chapter One – Quantum Chemistry Methods with Multiwavelet Bases on Massive Parallel Computers." *Annual Reports in Computational Chemistry*, December 2014, vol. 10, 3-24.

Zhang, Y.,* P. Balaprakash,* J. Meng,* V. Morozov,* S. Parker,* and K. Kumaran.* "Raexplore: Enabling Rapid, Automated Architecture Exploration for Full Applications." *Argonne Leadership Computing Facility Technical Report*, December 2014.

Abdel-Gawad, A. H., M. Thottethodi, and A. Bhatele. "RAHTM: Routing Algorithm Aware Hierarchical Task Mapping." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis,* November 2014, New Orleans, Louisiana, 325-335.

Dawson, W. and F. Gygi. "Optimized Scheduling Strategies for Hybrid Density Functional theory Electronic Structure Calculations." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*, November 2014, New Orleans, Louisiana, 685-692.

Liard, M., N. S. Martys, W. L. George, D. Lootens, and P. Hebraud. "Scaling Laws for the Flow of Generalized Newtonian Suspensions." *Journal of Rheology*, November 2014, vol. 58, 1993.

Nomura, K.-I., R. K. Kalia, A. Nakano, P. Vashishta, K. Shimamura, F. Shimojo, M. Kunaseth, P. C. Messina,* and N. A. Romero.* "Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*, November 2014, New Orleans, Louisiana, 661-673.

Rasquin, M.,* C. Smith, K. Chitale, E. S. Seol, B. A. Matthews, J. L. Martin, O. Sahni, R. M. Loy,* M. S. Shephard, and K. E. Jansen. "Scalable Implicit Flow Solver for Realistic Wing Simulations with Flow Control." *Computing in Science & Engineering*, November 2014, vol. 16, no. 6, 13-21.

Saghafian, A., L. Shunn, D. A. Philips, and F. Ham. "Large Eddy Simulations of the HIFiRE Scramjet Using a Compressible Flamelet/Progress Variable Approach." *Proceedings of the Combustion Institute*, November 2014.

Bazavov, A., C. Bernard, J. Komijani, C. M. Bouchard, C. DeTar, J. Foley, L. Levkova, D. Du, J. Laiho, A. X. El-Khadra, E. D. Freeland, E. Gámiz, S. Gottlieb, U. M. Heller, J. Kim, D. Toussaint, A. S. Kronfeld, P. B. Mackenzie, J. N. Simone, R. S. Van de Water, R. Zhou, E. T. Neil, and R. Sugar. "Charmed and Light Pseudoscalar Meson Decay Constants From Four-Flavor Lattice QCD with Physical Light Quarks." *Physical Review D*, October 2014, vol. 90, no. 074509.

Chatzopoulos, E., C. Graziani, and S. M. Couch. "Characterizing the Convective Fields in Massive Stars." *The Astrophysical Journal*, October 2014, vol. 795, no. 1.

Chekanov, S. V.,* E. May,* K. Strand, and P. Van Gemmeren.* "ProMC: Input-Output Data Format for HEP Applications Using Varint Encoding." *Computer Physics Communications*, October 2014, vol. 185, no. 10, 2629-2635.

Ghosh, P., J. R. Hammond,* S. Ghosh, and B. Chapman. "Performance Analysis of the NWChem TCE for Different Communication Patterns." *High Performance Computing Systems. Performance Modeling, Benchmarking and Simulation Lecture Notes in Computer Science*, October 2014, 281-294.

Green, J. R., J. W. Negele, A. V. Pochinsky, S. N. Syritsyn, M. Engelhardt, and S. Krieg. "Nucleon Electromagnetic Form Factors from Lattice QCD Using a Nearly Physical Pion Mass." *Physical Review D*, October 2014, vol. 90, no. 074507.

Freeman, G. S., J. P. Lequieu, D. M. Hinckley, J. K. Whitmer,* and J. J. de Pablo.* "DNA Shape Dominates Sequence Affinity in Nucleosome Formation." *Physical Review Letters*, October 2014, vol. 113, no. 168101.

Jansen, G. R., J. Engel, G. Hagen, P. Navratil, and A. Signoracci. "Ab Initio Coupled-Cluster Effective Interactions for the Shell Model: Application to Neutron-Rich Oxygen and Carbon Isotopes." *Physical Review Letters*, October 2014, vol. 113, no. 142502.

Lee, E.-J., P. Chen, and T. H. Jordan. "Testing Waveform Predictions of 3D Velocity Models Against Two Recent Los Angeles Earthquakes." *Seismological Research Letters*, October 2014, vol. 85, no. 6, 1275-1284.

Walker, J.,* E. Merzari,* A. Obabko,* P. Fischer,* and A. Siegel.* "Accurate Prediction of the Wall Shear Stress in Rod Bundles with the Spectral Element Method at High Reynolds Numbers." *International Journal of Heat and Fluid Flow*, October 2014.

Yi, H., M. Rasquin,* J. Fang, and I. A. Bolotnov. "In-Situ Visualization and Computational Steering for Large-Scale Simulation of Turbulent Flows in Complex Geometries." *2014 IEEE International Conference on Big Data*, October 2014, Washington, D.C., 567-572.

Aad, G. et al. (ATLAS Collaboration). "Search for High-Mass Dilepton Resonances in PP Collisions at s√=8 TeV with the ATLAS Detector." *Physical Review D*, September 2014, vol. 90, 052005.

Acun, B., A. Gupta, N. Jain, A. Langer, H. Menon, E. Mikida, X. Ni, M. Robson, Y. Sun, E. Totoni, L. Wesolowski, and L. Kale. "Parallel Programming with Migratable Objects: Charm++ in Practice." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*, September 2014, New Orleans, Louisiana, 647-658.

Bai, Z., N. H. Christ, T. Izubuchi, C. T. Sachrajda, A. Soni, and J. Yu. "KL-KS Mass Difference from Lattice QCD." *Physical Review Letters*, September 2014, vol. 113, no. 112003.

Caprio, M. A., P. Maris, and J. P. Vary. "Halo Nuclei He6 and He8 with the Coulomb-Sturmian Basis." *Physical Review C,* September 2014, vol. 90, no. 034305.

Di, S.,* L. Bautista-Gomez,* and F. Cappello.* "Optimization of Multi-Level Checkpoint Model with Uncertain Execution Scales." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*, September 2014, New Orleans, Louisiana, 907-918.

Dicaire, N. M., C. Omand, and P. Navrátil. "Alternative Similarity Renormalization Group Generators in Nuclear Structure Calculations." *Physical Review C*, September 2014, vol. 90, no. 034302.

Fodor, Z., K. Holland, J. Kuti, S. Mondal, D. Nogradi, and C.-H. Wong. "The Lattice Gradient Flow at Tree-Level and Its Improvement." *Journal of High Energy Physics*, September 2014.

Li, Z., X. Bian, B. Caswell, and G. E. Karniadakis. "Construction of Dissipative Particle Dynamics Models for Complex Fluids via the Mori-Zwanzig Formulation." *Soft Matter*, September 2014, vol. 10, 8659-8672.

Lifflander, J., E. Meneses, H. Menon, P. Miller, S. Krishnamoorthy, and L. V. Kale. "Scalable Replay with Partial-Order Dependencies for Message-Logging Fault Tolerance." *Proceedings of the Cluster Computing (CLUSTER) 2014 IEEE International Conference*, September 2014, Madrid, Spain, 19-28.

Phillips, C. L.* "A Learning Heuristic for Space Mapping and Searching Self-Organizing Systems Using Adaptive Mesh Refinement." *Journal of Computational Physics*, September 2014, vol. 272, no. 1, 799-813.

Phillips, J. C., Y. Sun, N. Jain, E. J. Bohm, and L. V. Kalé. "Mapping to Irregular Torus Topologies and Other Techniques for Petascale Biomolecular Simulation." *Proceedings of SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*, September 2014, New Orleans, Louisiana, 81-91.

Phillips, J. C., J. E. Stone, K. L. Vandivort, T. G. Armstrong, J. M. Wozniak,* M. Wilde,* and K. Schulten. "Petascale Tcl with NAMD, VMD, and Swift/T." *Proceedings of the 1st First Workshop for High Performance Technical Computing in Dynamic Languages*, September 2014, New Orleans, Louisiana, 6-17.

Wagner, L. K. and P. Abbamonte. "Effect of Electron Correlation on the Electronic Structure and Spin-Lattice Coupling of High-Tc Cuprates: Quantum Monte Carlo Calculations." *Physical Review B*, September 2014, vol. 90, no. 125129.

Yan, L. and H. Chen. "Migration of Holstein Polarons in Anatase TiO2." *Journal of Chemical Theory and Computation*, September 2014, vol. 10, no. 11, 4995-5001.

Alexeev, Y.,* D. G. Fedorov, and A. A. Shvartsburg. "Effective Ion Mobility Calculations for Macromolecules by Scattering on Electron Clouds." *The Journal of Physical Chemistry A*, August 2014, vol. 118, no. 34, 6763-72.

Böse, M., R. W. Graves, D. Gill, S. Callaghan, and P. J. Maechling. "CyberShake-Derived Ground-Motion Prediction Models for the Los Angeles Region with Application to Earthquake Early Warning." *Geophysical Journal International*, August 2014, vol. 198, no. 3, 1438-1457.

Elenewski, J. E. and H. Chen. "Real-Time Transport in Open Quantum Systems from PT-Symmetric Quantum Mechanics." *Physical Review B*, August 2014, vol. 90, no. 085104.

Hu, L., K. D. Hammond, B. D. Wirth, and D. Maroudas. "Dynamics of Small Mobile Helium Clusters Near Tungsten Surfaces." *Surface Science*, August 2014, vol. 626, L21-L25.

Lee, E.-J., P. Chen, T. H. Jordan, P. B. Maechling, M. Denolle, and G. C. Beroza. "Full-3-D Tomography for Crustal Structure in Southern California Based on the Scattering-Integral and the Adjoint-Wavefield Methods." *Journal of Geophysical Research*, August 2014.

Li, X., Z. Peng, H. Lei, M. Dao, and G. E. Karniadakis. "Probing Red Blood Cell Mechanics, Rheology and Dynamics with a Two-Component Multi-Scale Model." *Philosophical Transactions A*, August 2014, vol. 372.

McDonnell, J. D., W. Nazarewicz, J. A. Sheikh, A. Staszczak, and M. Warda. "Excitation-Energy Dependence of Fission in the Mercury Region." *Physical Review C*, August 2014, vol. 90, no. 021302(R).

Neuhauser, D., Y. Gao, C. Arntsen, C. Karshenas, E. Rabani, and R. Baer. "Breaking the Theoretical Scaling Limit for Predicting Quasiparticle Energies: The Stochastic GW Approach." *Physical Review Letters*, August 2014, vol. 113, no. 076402.

Pei, J. C. , G. I. Fann, R. J. Harrison, W. Nazarewicz, Y. Shi, and S. Thornton. "Adaptive Multi-Resolution 3D Hartree-Fock-Bogoliubov Solver for Nuclear Structure." *Physical Review C*, August 2014, vol. 90, no. 024317.

Restrepo, D. and J. Bielak. "Virtual Topography: A Fictitious Domain Approach for Analyzing Free-Surface Irregularities in Large-Scale Earthquake Ground Motion Simulation." *International Journal for Numerical Methods in Engineering*, August 2014.

Samara Technology Group, LLC. "Understanding the Scaling Behavior of the GFDL FMS High-Resolution Atmosphere Model on the Argonne BG/Q Platform." *Argonne Leadership Computing Facility Technical Report*, August 2014.

Savage, J. and G. A. Voth. "Persistent Subdiffusive Proton Transport in Perfluorosulfonic Acid Membranes." *The Journal of Physical Chemistry Letters*, August 2014, vol. 5, no. 17, 3037-3042.

Shi, Y., D. E. Ward, B. G. Carlsson, J. Dobaczewski, W. Nazarewicz, I. Ragnarsson, and D. Rudolph. "Structure of Superheavy Nuclei Along Decay Chains of Element 115." *Physical Review C*, August 2014, vol. 90, no. 014308.

Shirokov, A. M., A. G. Negoita, J. P. Vary, S. K. Bogner, A. I. Mazur, E. A. Mazur, and D. Gogny. "Properties of Nuclear Matter within the JISP16 NN Interaction." *Physical Review C*, August 2014, vol. 90, no. 024324.

Taborda, R. and J. Bielak. "Ground-Motion Simulation and Validation of the 2008 Chino Hills, California, Earthquake Using Different Velocity Models." *Bulletin of the Seismological Society of America*, August 2014, no. 104, 1876-1898.

Alfè, D., A. P. Bartók, G. Csányi, and M. J. Gillan. "Communication: Energy Benchmarking with Quantum Monte Carlo for Water Nano-Droplets and Bulk Liquid Water." *The Journal of Chemical Physics*, July 2014, vol. 138, no. 221102.

Alfè, D., A. P. Bartók, G. Csányi, and M. J. Gillan. "Analyzing the Errors of DFT Approximations for Compressed Water Systems." *The Journal of Chemical Physics*, July 2014, vol. 141, no. 1.

Borsanyi, S., Z. Fodor, S. D. Katz, S. Krieg, C. Ratti, and K. K. Szabo. "Freeze-Out Parameters from Electric Charge and Baryon Number Fluctuations: Is There Consistency?" *Physical Review Letters*, July 2014, vol. 113, no. 052301.

Deible, M. J., O. Tuguldur, and K. D. Jordan. "Theoretical Study of the Binding Energy of a Methane Molecule in a (H2O)20 Dodecahedral Cage." *The Journal of Physical Chemistry B*, July 2014, vol. 118, no. 28.

Maris, P., J. P. Vary, A. Calci, J. Langhammer, S. Binder, and R. Roth. "12C Properties with Evolved Chiral Three-Nucleon Interactions." *Physical Review C*, July 2014, vol. 90, no. 014314.

Ramakrishnan, R., P. O. Dral, M. Rupp, and O. A. von Lilienfeld.* "Quantum Chemistry Structures and Properties of 134 Kilo Molecules." *Scientific Data: Data Descriptor*, July 2014, vol. 1, no. 140022.

Romero-Redondo, C., S. Quaglioni, P. Navrátil, and G. Hupin. "He4+n+n Continuum Within an Ab Initio Framework." *Physical Review Letters*, July 2014, vol. 113, no. 032503.

Savage, J., Y.-L. S. Tse, and G. A. Voth. "Proton Transport Mechanism of Perfluorosulfonic Acid Membranes." *The Journal of Physical Chemistry C*, July 2014, 17436-17445.

Schuster, M. D., S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil. "Operator Evolution for Ab Initio Theory of Light Nuclei." *Physical Review C*, July 2014, vol. 90, no. 011301.

Vary, J. P. "Quantum Hamiltonian Physics with Supercomputers." *Nuclear Physics B - Proceedings Supplements*, July 2014, vol. 252-252, 155-164.

Vinuesa, R., A. Noorani, A. Lozano-Durán, G. K. El Khoury, P. Schlatter, P. F. Fischer,* and H. M. Nagib. "Aspect Ratio Effects in Turbulent Duct Flows Studied Through Direct Numerical Simulation." *Journal of Turbulence*, July 2014, vol. 15, no. 10, 677-706.

Wan, Q., L. Spanu, F. Gygi, and G. Galli. "Electronic Structure of Aqueous Sulfuric Acid from First-Principles Simulations with Hybrid Functionals." *The Journal of Physical Chemistry Letters*, July 2014, vol. 5, no. 15, 2562-2567.

Wang, J. and V. R. Kotamarthi.* "Downscaling With a Nested Regional Climate Model in Near-Surface Fields Over the Contiguous United States." *Journal of Geophysical Research Atmospheres*, July 2014, vol. 119, no. 14, 8778-8797.

Bailey, J. A., A. Bazavov, C. Bernard, C. M. Bouchard, C. DeTar, D. Du, A. X. El-Khadra, J. Foley, E. D. Freeland, E. Gámiz, S. Gottlieb, U. M. Heller, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, E. T. Neil, Si-Wei Qiu, J. Simone, R. Sugar, D. Toussaint, R. S. Van de Water, and R. Zhou. "Update of |Vcb| from the $B^{-} \to D^{-} \ell^{+} \nu^{-}$ Form Factor at Zero Recoil with Three-Flavor Lattice QCD." *Physical Review D*, June 2014, vol. 89, no. 114504.

Chen, H. "Functional Mode Electron-Transfer Theory." *The Journal of Physical Chemistry B*, June 2014, vol. 118, no. 27, 7586-7593.

Engel, M., P. F. Damasceno, C. L. Phillips,* and S. C. Glotzer. "Computational Self-Assembly of a One-Component Icosahedral Quasicrystal." *Nature Materials*, June 2014, vol. 14, 109-116.

Gaiduk, A. P., C. Zhang, F. Gygi, and G. Galli. "Structural and Electronic Properties of Aqueous NaCl Solutions from Ab Initio Molecular Dynamics Simulations with Hybrid Density Functionals." *Chemical Physical Letters*, June 2014, vol. 604, 89-96.

Green, J. R., M. Engelhardt, S. Krieg, J. W. Negele, A. V. Pochinsky, and S. N. Syritsyn. "Nucleon Structure from Lattice QCD Using a Nearly Physical Pion Mass." *Physical Review B*, June 2014, vol. 734, no. 27, 290-295.

Grote, M. J., J. Huber, D. Kourounis, and O. Sche. "Inexact Interior-Point Method for PDE-Constrained Nonlinear Optimization." *SIAM Journal on Scientific Computing*, June 2014, vol. 86, no. 3, 1251-1276.

Ham, F., D. Kim, S. Bose, H. Le, and M. Herrmann. "Simulation of Liquid Fuel Atomization by a Complex High-Shear Swirling Injector." *Proceedings of the ASME Turbo Expo 2014: Turbine Technical Conference and Exposition*, June 2014, Düsseldorf, Germany, vol. 4B, V04BT04A058.

Li, X., Y. H. Tang, H. Liang, and G. E. Karniadakis. "Large-Scale Dissipative Particle Dynamics Simulations of Self-Assembled Amphiphilic Systems." *Chemical Communications*, June 2014, vol. 50, 8306-8308.

Lopez-Bezanilla, A. and O. A. von Lilienfeld.* "Modeling Electronic Quantum Transport with Machine Learning." *Physical Review B*, June 2014, vol. 89, no. 235411.

Marom, N., T. Körzdörfer, X. Ren, A. Tkatchenko, and J. R. Chelikowsky. "Size Effects in the Interface Level Alignment of Dye-Sensitized TiO2 Clusters." *The Journal of Physical Chemistry Letters*, June 2014, vol. 5, no. 14, 2395-2401.

Rasquin, M.,* K. Chitale, M. Ali, and K. E. Jansen. "Parallel Adaptive Detached Eddy Simulations of the EUROLIFT DLR-F11 High Lift Configuration." *32nd AIAA Applied Aerodynamics Conference*, June 2014, Atlanta, Georgia.

Shimamura, K., F. Shimojo, R. K. Kalia, A. Nakano, K. Nomura, and P. Vashishta. "Hydrogen-on-Demand Using Metallic Alloy Nanoparticles in Water." *Nano Letters*, June 2014, vol. 14, no. 7, 4090-4096.

Somà, V., A. Cipollone, C. Barbieri, P. Navrátil, and T. Duguet. "Chiral Two- and Three-Nucleon Forces Along Medium-Mass Isotope Chains." *Physical Review C*, June 2014, vol. 89, no. 06130(R).

Alexeev, Y.,* S. Mickelson,* S. Leyffer,* R. Jacob,* and A. Craig. "The Heuristic Static Load-Balancing Algorithm Applied to the Community Earth System Model." *Proceedings of the 2014 IEEE International Parallel & Distributed Processing Symposium*, May 2014, Phoenix, Arizona, 1581-1590.

Binkowski, T. A.,* W. Jiang,* B. Roux, W. F. Anderson, and A. Joachimiak. "Virtual High-Throughput Ligand Screening." *Structural Genomics and Drug Discovery: Methods and Protocols*, May 2014, vol. 1140, 251-261.

Boyle, P. A., L. Del Debbio, N. Garron, R. J. Hudspith, E. Kerrane, K. Maltman, and J. M. Zanotti. "Combined NNLO Lattice-Continuum Determination of Lr10." *Physical Review D*, May 2014, vol. 89, no. 094510.

Clay III, R. C., J. Mcminis, J. M. McMahon, C. Pierleoni, D. M. Ceperley, and M. A. Morales. "Benchmarking Exchange-Correlation Functionals for Hydrogen at High Pressures Using Quantum Monte Carlo." *Physical Review B*, May 2014, vol. 89, no. 184106.

Dias, R. P., L. Li, T. A. Soares, and E. Alexov. "Modeling the Electrostatic Potential of Asymmetric Lipopolysaccharide Membranes: The MEMPOT Algorithm Implemented in DelPhi." *Computational Chemistry*, May 2014, vol. 35, no. 19, 1418-1429.

Dias, R. P., G. C. A. da Hora, M. Ramstedt, and T. A. Soares. "Outer Membrane Remodeling: The Structural Dynamics and Electrostatics of Rough Lipopolysaccharide Chemotypes." *Journal of Chemical Theory and Computation*, May 2014, vol. 10, no. 6, 2488-2497.

DiStasio Jr., R. A., B. Santra, Z. Li, X. Wu, and R. Car. "The Individual and Collective Effects of Exact Exchange and Dispersion Interactions on the Ab Initio Structure of Liquid Water." *The Journal of Chemical Physics*, May 2014, vol. 141, no. 084502.

Dorier, M., G. Antoniu, R. Ross,* D. Kimpe,* and S. Ibrahim.* "CALCioM: Mitigating I/O Interference in HPC Systems through Cross-Application Coordination." *Proceedings of the 2014 IEEE 28th International Parallel & Distributed Processing Symposium*, May 2014, Phoenix, Arizona, 155-164.

Kortelainen, M., J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich,* N. Schunck, S. M. Wild,* D. Davesne, J. Erler, and A. Pastore. "Nuclear Energy Density Optimization: Shell Structure." *Physical Review C*, May 2014, vol. 89, no. 054314.

Koziol, L. and M. M. Morales. "A Fixed-Node Diffusion Monte Carlo Study of the 1,2,3-Tridehydrobenzene Triradical." *The Journal of Chemical Physics*, May 2014, vol. 140, no. 224316.

Lia, Z., Y.-H. Tang, H. Lei, B. Caswell, and G. E. Karniadakis. "Energy-Conserving Dissipative Particle Dynamics with Temperature-Dependent Properties." *Journal of Computational Physics*, May 2014, vol. 265, 113-127.

Lovato, A.,* S. Gandolfi, J. Carlson, S. C. Pieper,* and R. Schiavilla. "Neutral Weak Current Two-Body Contributions in Inclusive Scattering from C12." *Physical Review Letters*, May 2014, vol. 112, no. 182502.

Mohr, S., L. E. Ratcliff, P. Boulanger, L. Genovese, D. Caliste, T. Deutsch, and S. Goedecker. "Daubechies Wavelets for Linear Scaling Density Functional Theory." *The Journal of Chemical Physics*, May 2014, vol. 140, no. 20.

Morales, M. A., J. R. Gergely, J. McMinis, J. M. McMahon, J. Kim, and D. M. Ceperley. "Quantum Monte Carlo Benchmark of Exchange-Correlation Functionals for Bulk Water." *Journal of Chemical Theory and Computation*, May 2014, vol. 10, no. 6, 2355-2362.

Petra, C.G.,* O. Schenk, and M. Anitescu.* "Real-Time Stochastic Optimization of Complex Energy Systems on High-Performance Computers." *Computing in Science & Engineering*, May 2014, 32-42.

Sheikh, J. A., N. Hinohara, J. Dobaczewski, T. Nakatsukasa, W. Nazarewicz, and K. Sato. "Isospin-Invariant Skyrme Energy-Density-Functional Approach with Axial Symmetry." *Physical Review C*, May 2014, vol. 89, no. 054317.

Shimojo, F., S. Hattori, R. K. Kalia, M. Kunaseth, W. Mou, A. Nakano, K. Nomura, S. Ohmura, P. Rajak, K. Shimamura, and P. Vashishta. "A Divide-Conquer-Recombine Algorithmic Paradigm for Large Spatiotemporal Quantum Molecular Dynamics Simulations." *Journal of Chemical Physics*, May 2014, vol. 140, no. 18, 18A529.

Smith, T. M., R. Van De Geijn, M. Smelyanskiy, J. R. Hammond,* and F. G. Van Zee. "Anatomy of High-Performance Many-Threaded Matrix Multiplication." *Proceedings of the 2014 IEEE 28th International Parallel & Distributed Processing Symposium*, May 2014, Phoenix, AZ, 1049-1059.

Tang, W., B. Wang, and S. Ethier. "Scientific Discovery in Fusion Plasma Turbulence Simulations at Extreme Scale." *Computing in Science & Engineering*, May 2014, vol. 16, no. 5, 44-52.

Upadhye, A.,* R. Biswas,* A. Pope,* K. Heitmann,* S. Habib,* H. Finkel,* and N. Frontiere.* "Large-Scale Structure Formation with Massive Neutrinos and Dynamical Dark Energy." *Physical Review D*, May 2014, vol. 89, no. 10, 103515.

Zheng, Y., A. Kamil, M. B. Driscoll, H. Shan, and K. Yelick. "UPC++: A PGAS Extension for C++." *Proceedings of the 2014 IEEE 28th International Parallel & Distributed Processing Symposium*, May 2014, Phoenix, Arizona, 1105-1114.

Beane, S. R., S. D. Cohen, W. Detmold, H.-W. Lin, and M. J. Savage. "Nuclear σ Terms and Scalar-Isoscalar WIMP-Nucleus Interactions from Lattice QCD." *Physical Review D,* April 2014, vol. 89.

Couch, S. M., and E. P. O'Connor. "High-Resolution Three-Dimensional Simulations of Core-Collapse Supernovae in Multiple Progenitors." *The Astrophysical Journal*, April 2014, vol. 785, no. 2.

Forbes, M. M., A. Gezerlis, K. Hebeler, T. Lesinski, and A. Schwenk. "Neutron Polaron as a Constraint on Nuclear Density Functionals." *Physical Review C*, April 2014, vol. 89, no. 04130.

Heitmann, K.,* S. Habib,* H. Finkel,* N. Frontiere,* A. Pope,* V. Morozov,* E. R. E. Kovacs,* J. Kwan,* L. Nan,* S. Rizzi,* J. Insley,* V. Vishwanath,* T. Peterka,* D. Daniel, P. Fasel, and G. Zagaris. "Large Scale Simulations of Sky Surveys." *Computing in Science & Engineering*, April 2014, vol. 16, no. 5, 14-23.

Jiang, T., K. J. Evans, Y. Deng, and X. Dong. "Intermediate Frequency Atmospheric Disturbances: A Dynamical Bridge Connecting Western U.S. Extreme Precipitation with East Asian Cold Surges." *Journal of Geophysical Research*, April 2014, vol. 119, no. 7, 3723-3735.

Lee, M., R. Ulerich, N. Malaya, and R. D. Moser. "Experiences from Leadership Computing in Simulations of Turbulent Fluid Flows." *Computing in Science & Engineering*, April 2014, vol. 16, no. 5, 24-31.

Roten, D., K. B. Olsen, S. M. Day, Y. Cui, and D. Fäh. "Expected Seismic Shaking in Los Angeles Reduced by San Andreas Fault Zone Plasticity." *Geophysical Research Letters*, April 2014, vol. 41, no. 8, 2769-2777.

Wang, F. and T. H. Jordan. "Comparison of Probabilistic Seismic-Hazard Models Using Averaging-Based Factorization." *Bulletin of the Seismological Society of America*, April 2014.

Balantekin, A. B., J. Carlson, D. J. Dean, G. M. Fuller, R. J. Furnstahl, M. Hjorth-Jensen, R. V. F. Janssens,* B.-A. Li, W. Nazarewicz, F. M. Nunes, W. E. Ormand, S. Reddy, and B. M. Sherrill. "Nuclear Theory and Science of the Facility for Rare Isotope Beams." *Modern Physics Letters A*, March 2014, vol. 29, no. 11.

Bazavov, A., C. Bernard, C. M. Bouchard, C. DeTar, D. Du, A. X. El-Khadra, J. Foley, E. D. Freeland, E. Gámiz, S. Gottlieb, U. M. Heller, J. Kim, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, E. T. Neil, M. B. Oktay, Si-Wei Qiu, J. N. Simone, R. Sugar, D. Toussaint, R. S. Van de Water, and R. Zhou. "Determination of |Vus| from a Lattice QCD Calculation of the K→πℓν Semileptonic Form Factor with Physical Quark Masses." *Physical Review Letters*, March 2014, vol. 112, no. 112001.

Derya, V., D. Savran, J. Endres, M. N. Harakeh, H. Hergert, J. H. Kelleyg, P. Papakonstantinou, N. Pietralla, V. Y. Ponomarev, R. Roth, G. Rusevk, A. P. Tonchevk, W. Tornowk, H. J. Wörtched, and A. Zilgesa. "Isospin Properties of Electric Dipole Excitations in 48Ca." *Physical Review B*, March 2014, vol. 730, 288-292.

Gandolfi, S. and A. W. Steiner. "From Nuclear Structure to Neutron Stars." *INPC 2013 – International Nuclear Physics Conference*, March 2014, vol. 66, 01017.

Gleizer, A., G. Peralta, J. R. Kermode, A. De Vita, and D. Sherman. "Dissociative Chemisorption of O2 Inducing Stress Corrosion Cracking in Silicon Crystals." *Physical Review Letters*, March 2014, vol. 112, no. 11, 115501.

Gordillo, T. R., S. Sharifzadeh, L. Kronik, and J. Neaton. "Understanding Singlet and Triplet Excitons in Acene Crystals from First Principles." *Bulletin of the American Physical Society*, March 2014, vol. 59, no. 1.

Hammond, J. R.,* S. Ghosh, and B. M. Chapman. "Implementing OpenSHMEM Using MPI-3 One-Sided Communication." *OpenSHMEM and Related Technologies: Experiences, Implementations, and Tools Lecture Notes in Computer Science*, March 2014, 44-58.

Ilsche, T., J. Schuchart, J. Cope,* D. Kimpe,* T. Jones, A. Knüpfer, K. Iskra,* R. Ross,* W. E. Nagel, and S. Poole. "Optimizing I/O Forwarding Techniques for Extreme-Scale Event Tracing." *Cluster Computing*, March 2014, vol. 17, no. 1, 1-18.

Jackson, A. P., D. M. Townsley, and A. C. Calder. "Power-Law Wrinkling Turbulence-Flame Interaction Model for Astrophysical Flames." *The Astrophysical Journal*, March 2014, vol. 784, no. 2.

Kim, C. and G. E. Karniadakis. "Microscopic Origin of Drag Force: A New Mathematical and Physical Interpretation." *Bulletin of the American Physical Society*, March 2014, vol. 59, no. 1.

Meehl, G. A. and H. Teng. "CMIP5 Multi-Model Hindcasts for the Mid-1970s Shift and Early 2000s Hiatus and Predictions for 2016-2035." *Geophysical Research Letter*, March 2014, vol. 41, no. 5, 1711-1716.

Meier, K., T. Laino, and A. Curioni. "Solid-State Electrolytes: Revealing the Mechanisms of Li-Ion Conduction in Tetragonal and Cubic LLZO by First-Principles Calculations." *The Journal of Physical Chemistry C*, March 2014, vol. 118, no. 13, 6668-6679.

Nadvorny, D., J. Bosco, P. da Silva, and R. D. Lins. "Anionic Form of Usnic Acid Promotes Lamellar to Nonlamellar Transition in DPPC and DOPC Membranes." *The Journal of Physical Chemistry B*, March 2014, vol. 118, no. 14, 3881-3886.

Roberts, N. V., T. Bui-Thanh, and L. Demkowicz. "The DPG Method for the Stokes Problem." *Computers & Mathematics with Applications*, March 2014, vol. 67, no. 4, 966-995.

Sharifzadeh, S., C. Wong, H. Wu, N. Ginsberg, L. Kroni, and J. Neaton. "Understanding the Role of Orientational Heterogeneity on Photophysical Properties of Organic Polycrystalline Films." *Bulletin of the American Physical Society*, March 2014, vol. 59, no. 1.

Ambrosetti, A., D. Alfe, R. A. DiStasio, Jr., and A. Tkatchenko. "Hard Numbers for Large Molecules: Toward Exact Energetics for Supramolecular Systems." *The Journal of Physical Chemistry Letters*, February 2014, vol. 5, no. 5, 849-855.

Bui, H., H. Finkel,* V. Vishwanath,* S. Habib,* K. Heitmann,* J. Leigh, M. E. Papka,* and K. Harms.* "Scalable Parallel I/O on a Blue Gene/Q Supercomputer Using Compression, Topology-Aware Data Aggregation, and Subfiling." *Proceedings of the 22nd Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP 2014)*, February 2014, Turin, Italy, 107-111.

Chitale, K., M. Rasquin,* O. Sahni, M. Shephard, and K. Jansen. "Anisotropic Boundary Layer Adaptivity of Multi-Element Wings." *52nd Aerospace Sciences Meeting*, February 2014, National Harbor, Maryland.

Chitale, K., M. Rasquin,* J. Martin, and K. Jansen. "Finite Element Flow Simulations of the EUROLIFT DLR-F11 High Lift Configuration." *52nd Aerospace Sciences Meeting*, February 2014, National Harbor, Maryland.

Dobaczewski, J., W. Nazarewicz, and P.-G. Reinhard. "Error Estimates of Theoretical Models: A Guide." *Journal of Physics G: Nuclear and Particle Physics*, February 2014, vol. 41, no. 074001.

Gandolfi, S., J. Carlson, S. Reddy, A. W. Steiner, and R. B. Wiringa.* "The Equation of State of Neutron Matter, Symmetry Energy and Neutron Star Structure." *The European Physical Journal A*, February 2014, vol. 50, no. 2.

Lifflander, J., P. Miller, and L. Kale. "Adoption Protocols for Fanout-Optimal Fault-Tolerant Termination Detection." *Proceedings of the 18th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*, February 2014, vol. 48, no. 8, 13-22.

Lovato, A.,* O. Benhar, S. Gandolfi, and C. Losa. "Neutral-Current Interactions of Low-Energy Neutrinos in Dense Neutron Matter." *Physical Review C*, February 2014, vol. 89, no. 025804.

Meehl, G. A., L. Goddard, G. Boer, R. Burgman, G. Branstator, C. Cassou, S. Corti, G. Danabasoglu, F. Doblas-Reyes, E. Hawkins, A. Karspeck, M. Kimoto, A. Kumar, D. Matei, J. Mignot, R. Msadek, A. Navarra, H. Pohlmann, M. Rienecker, T. Rosati, E. Schneider, D. Smith, R. Sutton, H. Teng, G. J. van Oldenborgh, G. Vecchi, and S. Yeager. "Decadal Climate Prediction: An Update from the Trenches." *Bulletin of the American Meteorological Society*, February 2014, vol. 95, no. 2.

Nazarewicz, W., P.-G. Reinhard, W. Satuła, and D. Vretenar. "Symmetry Energy in Nuclear Density Functional Theory." *The European Physical Journal A*, February 2014, vol. 50, no. 2.

Poulson, J., L. Demanet, N. Maxwell, and L. Ying. "A Parallel Butterfly Algorithm." *SIAM Journal on Scientific Computing*, February 2014, vol. 36, no. 1, C49-C65.

Wang, J.,* Y. Han, R. Kotamarthi, and M. L. Stein. "Nested Regional Climate Model (NRCM) Downscaling in Extreme Temperature: Evaluated by Generalized Extreme Value (GEV) Distribution." *Proceedings of the 26th Conference on Climate Variability and Change*, February 2014, Atlanta, Georgia.

Wiringa, R. B.,* R. Schiavilla, S. C. Pieper,* and J. Carlson. "Nucleon and Nucleon-Pair Momentum Distributions in A≤12 Nuclei." *Physical Review C*, February 2014, vol. 89, 024305.

Alexeev, Y.,* M. P. Mazanetz, O. Ichihara, and D. G. Fedorov. "GAMESS as a Free Quantum-Mechanical Platform for Drug Research." *Current Topics in Medicinal Chemistry*, January 2014, vol. 12, no. 18.

Bose, S. T. and P. Moin. "A Dynamic Slip Boundary Condition for Wall-Modeled Large-Eddy Simulation." *Physics of Fluids*, January 2014, vol. 26, 015104.

Branstator, G. and H. Teng. "Is AMOC More Predictable than North Atlantic Heat Content?" *Journal of Climate*, January 2014, vol. 27, 3537-3550.

Ferraris, C. F., N. S. Martys, and W. L. George. "Development of Standard Reference Materials for Rheological Measurements of Cement-Based Materials." *Cement & Concrete Composites*, January 2014, vol. 54, 29-33.

Gandolfi, S. "Quantum Monte Carlo Study of Strongly Interacting Fermi Gases." *Journal of Physics: Conference Series*, January 2014, vol. 529.

Hagen, G., T. Papenbrock, A. Ekström, K. A. Wendt, G. Baardsen, S. Gandolfi, M. Hjorth-Jensen, and C. J. Horowitz. "Coupled-Cluster Calculations of Nucleonic Matter." *Physical Review C*, January 2014, vol. 89, no. 014319.

Hammond, K. D. and B. D. Wirth. "Crystal Orientation Effects on Helium Ion Depth Distributions and Adatom Formation Processes in Plasma-Facing Tungsten." *The Journal of Applied Physics*, January 2014, vol. 116, no. 143301.

Hu, L., K. D. Hammond, B. D. Wirth, and D. Maroudas. "Interactions of Mobile Helium Clusters with Surfaces and Grain Boundaries of Plasma-Exposed Tungsten." *The Journal of Applied Physics*, January 2014, vol. 115, no. 173512.

Huchette, J., M. Lubin, and C. Petra.* "Parallel Algebraic Modeling for Stochastic Optimization." *Proceedings of the 1st First Workshop for High Performance Technical Computing in Dynamic Languages*, January 2014, 29-35.

Kermode, J., G. Peralta, Z. Lia, and A. De Vita. "Multiscale Modelling of Materials Chemomechanics: Brittle Fracture of Oxides and Semiconductors." *Procedia Materials Science,* January 2014, vol. 3, 1681-1686.

Kim, C. and G. E. Karniadakis. "Time Correlation Functions of Brownian Motion and Evaluation of Friction Coefficient in the Near-Brownian-Limit Regime." *Multiscale Modeling and Simulation*, January 2014, vol. 12, no. 1, 225-248.

Kruppa, A. T., G. Papadimitriou, W. Nazarewicz, and N. Michel. "Nuclear Three-Body Problem in the Complex Energy Plane: Complex-Scaling Slater Method." *Physical Review C*, January 2014, vol. 89, 014330.

Lonardoni, D., F. Pederiva, and S. Gandolfi. "Accurate Determination of the Interaction Between Λ Hyperons and Nucleons from Auxiliary Field Diffusion Monte Carlo Calculations." *Physical Review C*, January 2014, vol. 89, no. 014314.

Lopez-Bezanilla, A.* "Electronic and Quantum Transport Properties of Substitutionally Doped Double-Walled Carbon Nanotubes." *The Journal of Physical Chemistry C*, January 2014, vol. 118, no. 3, 1472-1477.

May, J., J. Tonge, I. Ellis, W. B. Mori, F. Fiuza, R. A. Fonseca, L. O. Silva, and C. Ren. "Enhanced Stopping of Macro-Particles in Particle-in-Cell Simulations." *Physics of Plasmas*, January 2014, vol. 21, no. 052703.

Park, G. I. and P. Moin. "An Improved Dynamic Non-Equilibrium Wall-Model for Large Eddy Simulation." *Physics of Fluids*, January 2014, vol. 26, 015108.

Petra, C. G.,* O. Schenk, M. Lubin, and K. Gäertner. "An Augmented Incomplete Factorization Approach for Computing the Schur Complement in Stochastic Optimization." *SIAM Journal on Scientific Computing*, January 2014, vol. 36, no. 2, 139-162.

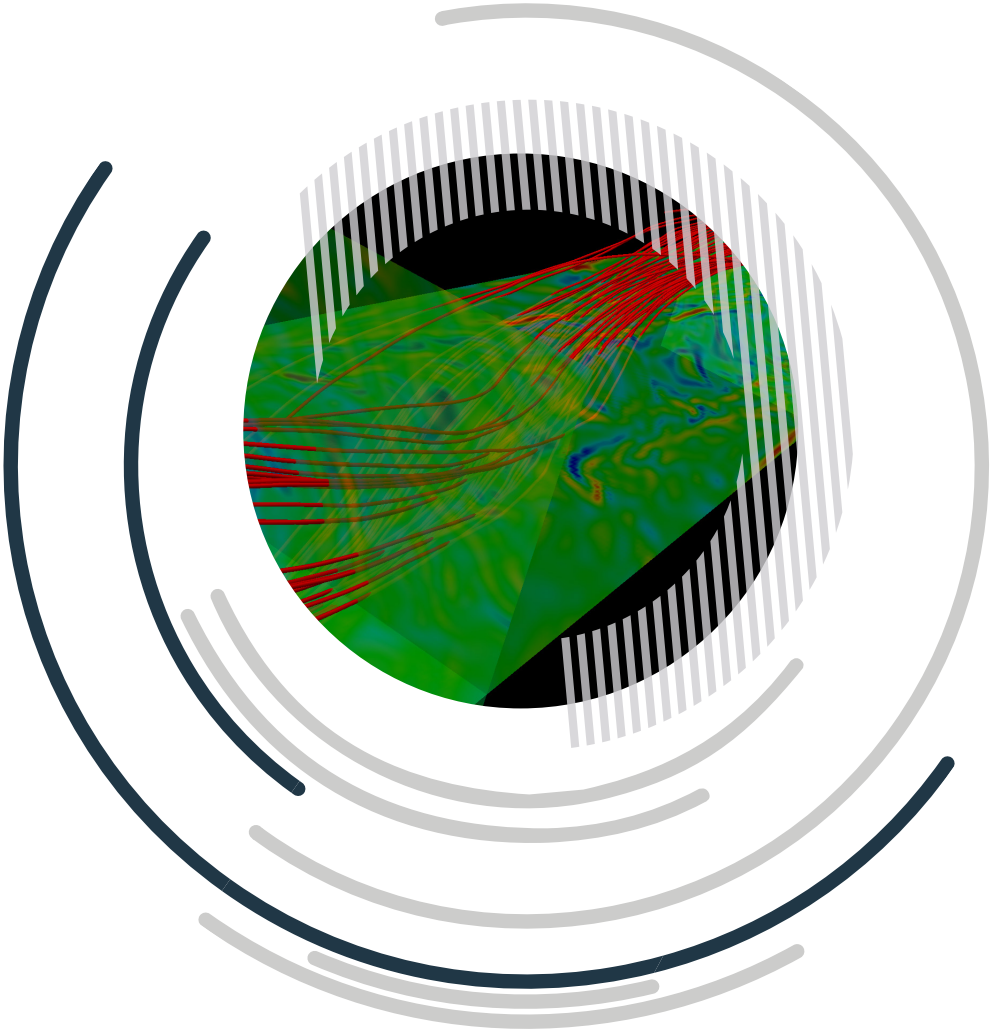
Poyraz, E., H. Xu, and Y. Cui. "Application-Specific I/O Optimizations on Petascale Supercomputers." *Procedia Computer Science*, January 2014, vol. 29, 910-923.

Saidi, W. A. and N. Patrick. "Probing Single-Walled Carbon Nanotube Defect Chemistry Using Resonance Raman Spectroscopy." *Carbon*, January 2014, vol. 67, 17-26.

Shin, H., S. Kang, J. Koo, H. Lee, J. Kim, and Y. Kwon. "Cohesion Energetics of Carbon Allotropes: Quantum Monte Carlo Study." *The Journal of Chemical Physics*, January 2014, vol. 140, no. 114702.

Wallace, S.,* V. Vishwanath,* S. Coghlan,* J. Tramm,* Z. Lan, and M. E. Papka.* "Application Power Profiling on IBM Blue Gene/Q." *Proceedings of the Cluster Computing (CLUSTER) 2013 IEEE International Conference*, January 2014, Indianapolis, Indiana, 1-8.

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

SiO2 Fracture: Chemo-mechanics with a Machine Learning Hybrid QM/MM Scheme
James Kermode, University of Warwick
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

Large-Scale Quantum Simulations of Electrode-Electrolyte Interfaces
Giulia Galli, University of Chicago
Allocation: 35 Million Core-Hours

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

Revealing the Reversible Electrodeposition Mechanism in Multivalent-Ion Batteries
Gerbrand Ceder, Massachusetts Institute of Technology
Allocation: 98 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

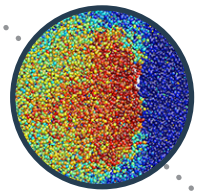
Physics

Calculation of Nuclear Matrix Element of Neutrinoless Double-Beta Decay
Jun Terasaki, University of Tsukuba
Allocation: 6.6 Million Core-Hours

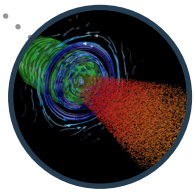
Cosmic Reionization on Computers
Nickolay Y. Gnedin, Fermilab/University of Chicago
Allocation: 3.5 Million Core-Hours

Grid-Enabling High-Performance Computing for ATLAS
Thomas J. LeCompte, Argonne National Laboratory
Allocation: 3.1 Million Core-Hours

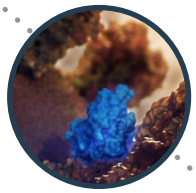
FEATURED IMAGES



Visualization taken from an 8-million-atom molecular dynamics simulation of a shockwave interacting with a 20 nm cylindrical void in a molecular crystal of high explosive PETN, causing the void to collapse. Image credit: Tzu-Ray Shan and Aidan Thompson, Sandia National Laboratories



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



Researchers in the Baker lab at the University of Washington have computationally designed a novel protein (blue) that binds to the base of hemagglutinin (orange) and effectively neutralizes the flu virus. Image credit: Vikram K. Mulligan, University of Washington

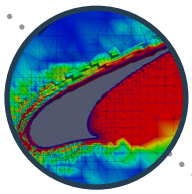
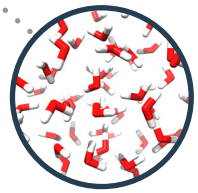
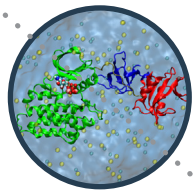


Illustration of mesh adaptation with a slice through the mesh of a three element high lift wing (slat and main wing view). Image credit: Kenneth Jansen, University of Colorado

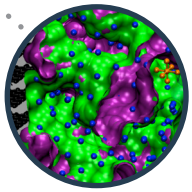


The surface affinity of ions in aqueous solution can have a profound effect on the chemistry in a range of atmospheric phenomena. Image credit: Spencer R. Pruitt, Argonne National Laboratory

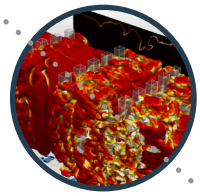


The Src-family of kinases are important enzymes for cellular signaling that can transfer a phosphoryl group from ATP to a target protein. Image credit: Avisek Das, Mikolai Fajer, and Benoît Roux, University of Chicago

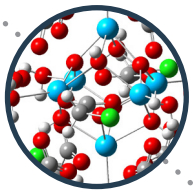
Electronic structure simulations of solvated molecular and atomic species near Pt(111) transition metal surfaces. Image credit: Jeffrey Greeley, Purdue University



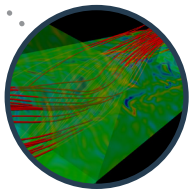
Equilibrated interface from atomistic simulations between a solid electrolyte interphase consisting of lithiated components and electrolyte. Image credit: Ryan Jorn, Argonne National Laboratory/University of Chicago



Large eddy simulation of an explosion in a venting chamber. Image credit: David Barré, CERFACS



Density functional theory-optimized structure for $Th_6(OH)_4O_4(H_2O)_6(ClCH_2COO)_{12}$. Image credit: Karah Knope and Lynne Soderholm, Argonne National Laboratory; David Dixon and Monica Vasiliu, University of Alabama



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

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.

AVAILABILITY OF THIS REPORT (ANL/ALCF-15/1)

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/).

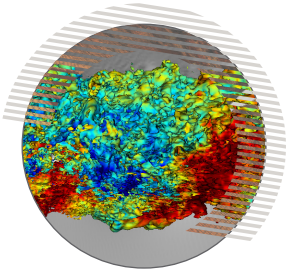
Reports not in digital format may be purchased by the public from the National Technical Information Service (NTIS):

U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandra, VA 22312
www.ntis.gov
phone | 800.553.NTIS (6847) or 703.605.6000
fax | 703.605.6900
orders@ntis.gov

Reports not in digital format are available to DOE and DOE contractors from the Office of Scientific and Technical Information (OSTI):

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone | 865.576.8401
fax | 865.576.5728
reports@adonis.osti.gov

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



U.S. DEPARTMENT OF ENERGY

Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

alcf_annual_report2014_rc