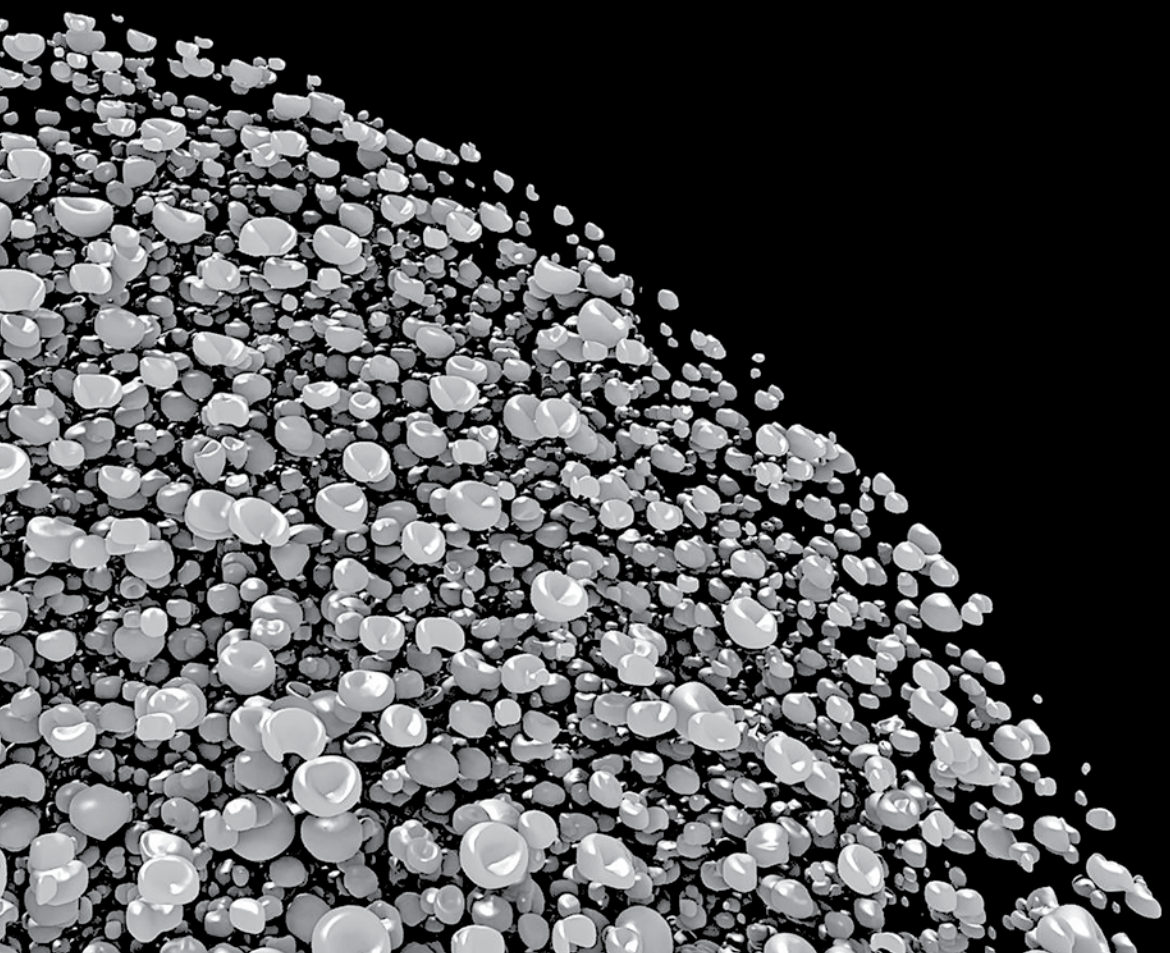
Argonne NATIONAL LABORATORY

2016 SCIENCE

ARGONNE LEADERSHIP COMPUTING FACILITY



On the cover Collapse of spherical cloud with 50,000 bubbles. The generation of microjets directed toward the cloud center causes the formation of cap-like bubble shapes.

Image credit: Computational Science and Engineering Laboratory, ETH Zürich, Switzerland

ARGONNE LEADERSHIP COMPUTING FACILITY

2016 SCIENCE HIGHLIGHTS

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ABOUT ALCF

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

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

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

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

Visualization of the deflagration-to-detonation transition of an explosive material from a 1-billion particle simulation conducted with the Uintah computational framework.

Image credit: Jacqueline Beckvermit and Martin Berzins, University of Utah

SCIENCE DIRECTOR'S MESSAGE

Katherine Riley
ALCF Director of Science

In my first full year as Director of Science, I've had a front row seat to the important work being done by our user community. This annually published collection of science highlights showcases some of the most exciting advancements and tools that have come into being over the past year with the help of our world-class resources and scientific computing staff.

The range of achievements you will read about here are as diverse as our community itself. Perhaps the single unifying thread that defines this unique group is that they all push the boundaries of their fields. Here are some examples:

- An Argonne team is using Mira to demonstrate how supercomputers can drastically quicken the pace of discoveries at large-scale physics experiments, such as CERN's Large Hadron Collider.
- Researchers from the University of Colorado Boulder are using simulations to understand how airplane wings equipped with synthetic air jets affect drag and fuel efficiency.
- A Brown University team is using Mira to better understand a life-threatening medical condition called thoracic aortic aneurysm and dissection.
- Argonne computational scientists have teamed up with experimentalists to use simulation results from Mira to design a self-healing coating material that significantly reduces friction in engines.

In 2016, we launched the ALCF Data Science Program, as well as an ALCF team dedicated to supporting complex workflows and data-intensive needs. It's an exciting time for leadership computing as our workload continues to evolve toward new use models that involve real-time data analysis, deep learning methods, and tighter coupling with experiment. With our data science program and team in place, we are exploring and improving the computational tools and techniques needed to fuel a new era of data-driven discoveries.

Last, but certainly not least, Theta arrived at Argonne this summer. The system has been installed and is currently being deployed. Our Early Science project teams will get the first chance to take advantage of Theta's advanced capabilities as they pursue ambitious research goals that range from modeling the brain to simulating the universe. Theta will serve as a bridge to our next-generation supercomputer, Aurora, which is scheduled for delivery in 2018.

We'll soon be announcing the selected projects for Aurora's Early Science Program. With two Early Science Programs underway and our involvement in more than a half-dozen Exascale Computing Program Application programs, we have a lot to look forward to in 2017.

ALLOCATION PROGRAMS

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

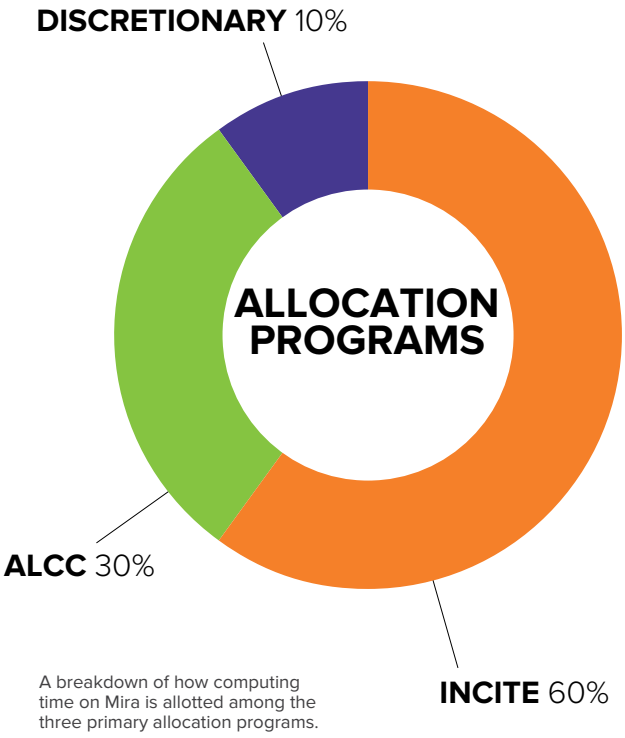
The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering.

ASCR Leadership Computing Challenge (ALCC)

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

Director's Discretionary

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



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

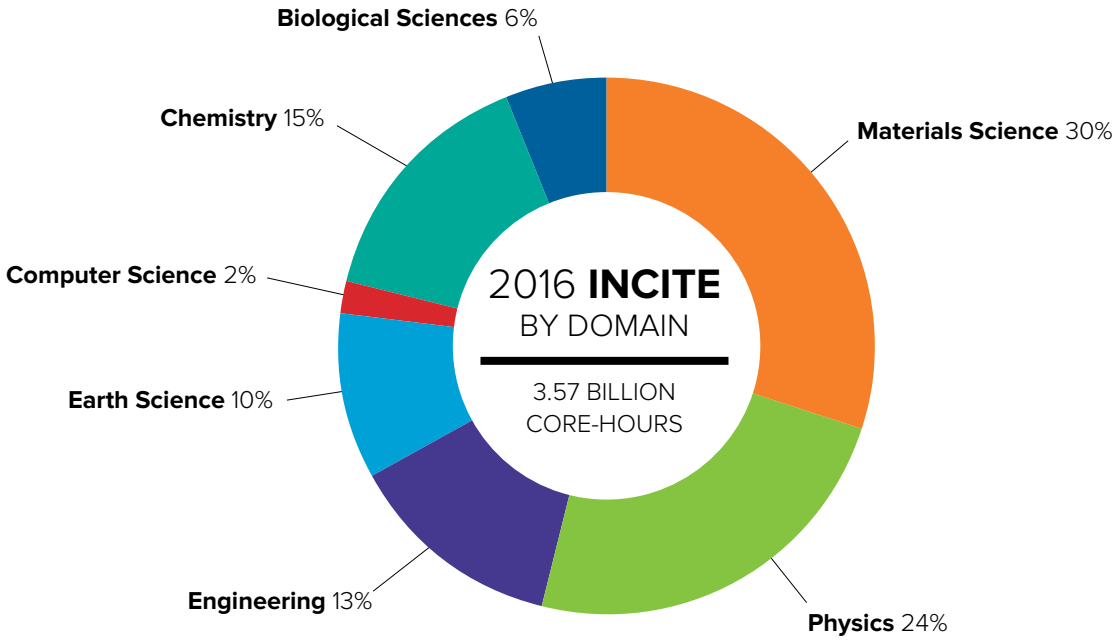
APPLICATION PROGRAMS

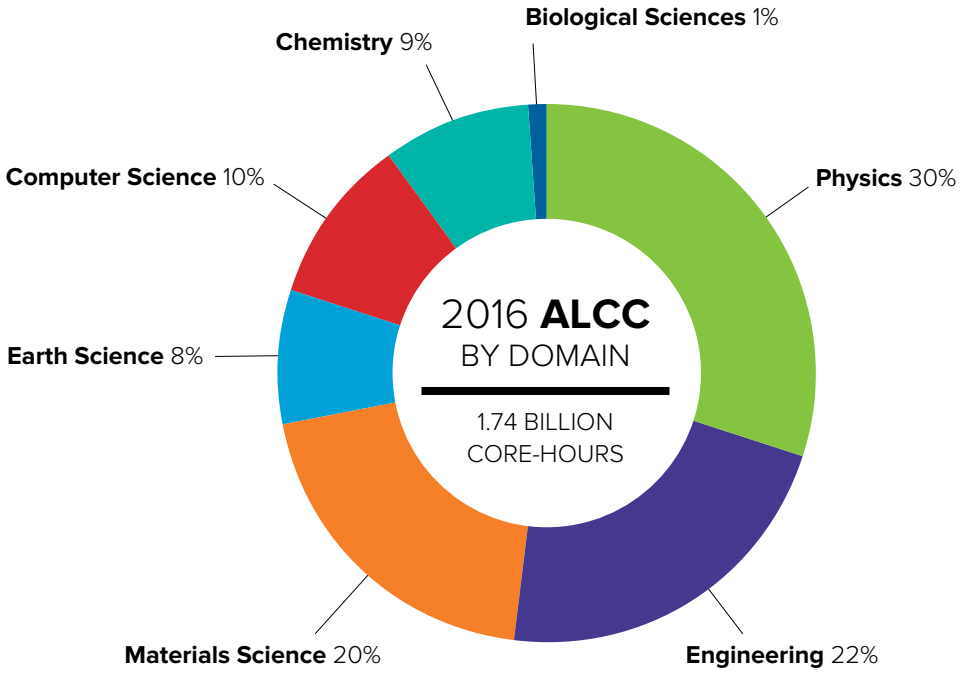
Early Science Program (ESP)

As part of the process of bringing a new supercomputer into production, the ALCF hosts the ESP to ensure its next-generation systems are ready to hit the ground running.

ALCF Data Science Program (ADSP)

ADSP is targeted at big data science problems that require the scale and performance of leadership computing resources.





Note: ALCC data is from calendar year 2016.

PREPARING FOR FUTURE PLATFORMS

Leading-edge computing technologies are intrinsic to the ALCF. The facility is continually working to develop tools and approaches that will support and enable forefront computational research on the systems of the future.

DEVELOPING CAPABILITIES FOR NEXT-GENERATION SYSTEMS

Established by the ALCF and Argonne's Mathematics and Computer Science Division, the Joint Laboratory for System Evaluation (JLSE) provides laboratory researchers with access to leading-edge computing resources to enable the development of capabilities that will improve science productivity on future hardware and software platforms.

The JLSE also provides an avenue for Argonne researchers to work collaboratively with HPC vendors on prototype technologies for petascale and beyond.

The following summaries represent a selection of current JLSE projects.

RAN – RAM Area Network

William E. Allcock

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

Evaluation of Neuromorphic Computing Hardware

Hal Finkel, Fangfang Xia

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

Testing Globus with Spectra Logic BlackPearl

Ian Foster

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

Petrel Data Service Testbed

Ian Foster, Michael E. Papka

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

Integration and Validation of Argo's Components

Swann Perarnau

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

ALCF Theta Early Science Program

Tim Williams

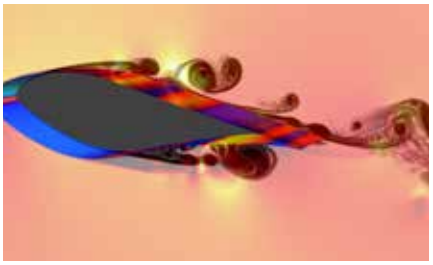
Theta Early Science Program teams are using JLSE resources to prepare and optimize applications for Theta in advance of the system being available.

READYING THETA FOR SCIENCE ON DAY ONE

As part of the process of bringing a new supercomputer into production, the ALCF conducts the Early Science Program (ESP) to ensure its next-generation systems are ready to hit the ground running. The intent of the ESP is to use the critical pre-production time period to prepare key applications for the architecture and scale of a new supercomputer, and to solidify libraries and infrastructure to pave the way for other production applications to run on the system.

For the Theta ESP, six Tier 1 projects were selected to optimize applications for Theta while pursuing ambitious science goals on the system. An additional six Tier 2 projects were selected for code development work.

TIER 1 PROJECTS

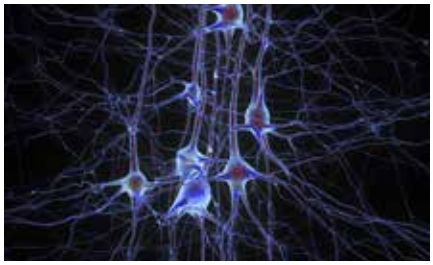


Scale-Resolving Simulations of Wind Turbines with SU2

Juan J. Alonso
Stanford University

Code: SU2

Alonso's team is developing a simulation capability that will help inform the design of improved wind turbines and large wind farms.

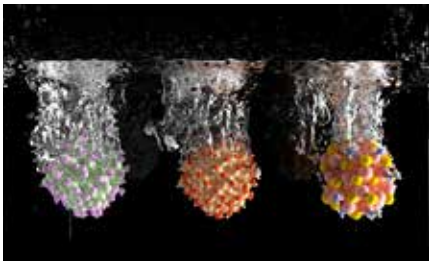


Large-Scale Simulation of Brain Tissue: Blue Brain Project, EPFL

Fabien Delalondre
Ecole Federale Polytechnique de Lausanne

Code: CoreNeuron

Delalondre's project involves simulating brain plasticity—experience-dependent changes in synaptic connectivity—to improve our understanding of the brain.



First-Principles Simulations of Functional Materials for Energy Conversion

Giulia Galli
The University of Chicago/Argonne National Laboratory

Codes: Qbox, WEST

Galli's team is developing simulation methods to optimize properties of nanostructured materials for use in solar and thermal energy conversion devices.

TIER 2 PROJECTS

Electronic Structure-Based Discovery of Hybrid Photovoltaic Materials on Next-Generation HPC Platforms

Volker Blum
Duke University

Codes: FHI-aims, GAtor

Flow, Mixing, and Combustion of Transient Turbulent Gaseous Jets in Confined Cylindrical Geometries

Christos Frouzakis
Swiss Federal Institute of Technology Zurich

Code: Nek5000

Advanced Electronic Structure Methods for Heterogeneous Catalysis and Separation of Heavy Metals

Mark Gordon
Iowa State University

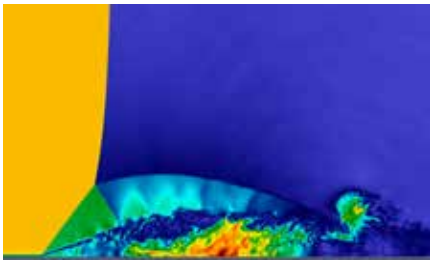
Code: GAMESS

Next-Generation Cosmology Simulations with HACC: Challenges from Baryons

Katrin Heitmann
Argonne National Laboratory

Code: HACC

Heitmann's project aims to further our understanding of astrophysical processes by performing detailed simulations of the universe for comparison with the latest observational data.

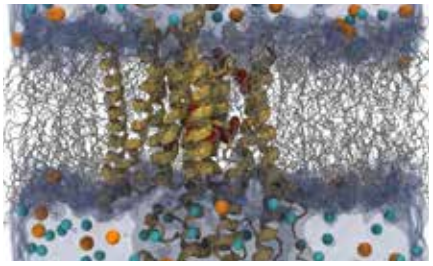


Direct Numerical Simulations of Flame Propagation in Hydrogen-Oxygen Mixtures in Closed Vessels

Alexei Khokhlov
The University of Chicago

Code: HSCD

Khokhlov's team is performing direct numerical simulations to better understand flame acceleration and the deflagration-to-detonation transition process in hydrogen-oxygen mixtures in closed spherical vessels.



Free Energy Landscapes of Membrane Transport Proteins

Benoît Roux
The University of Chicago/Argonne National Laboratory

Code: NAMD

Roux's team is carrying out simulations to provide an atomistic picture of membrane transport proteins, which will improve our understanding of a broad range of biological functions.

Extreme-Scale Unstructured Adaptive CFD: From Multiphase Flow to Aerodynamic Flow Control

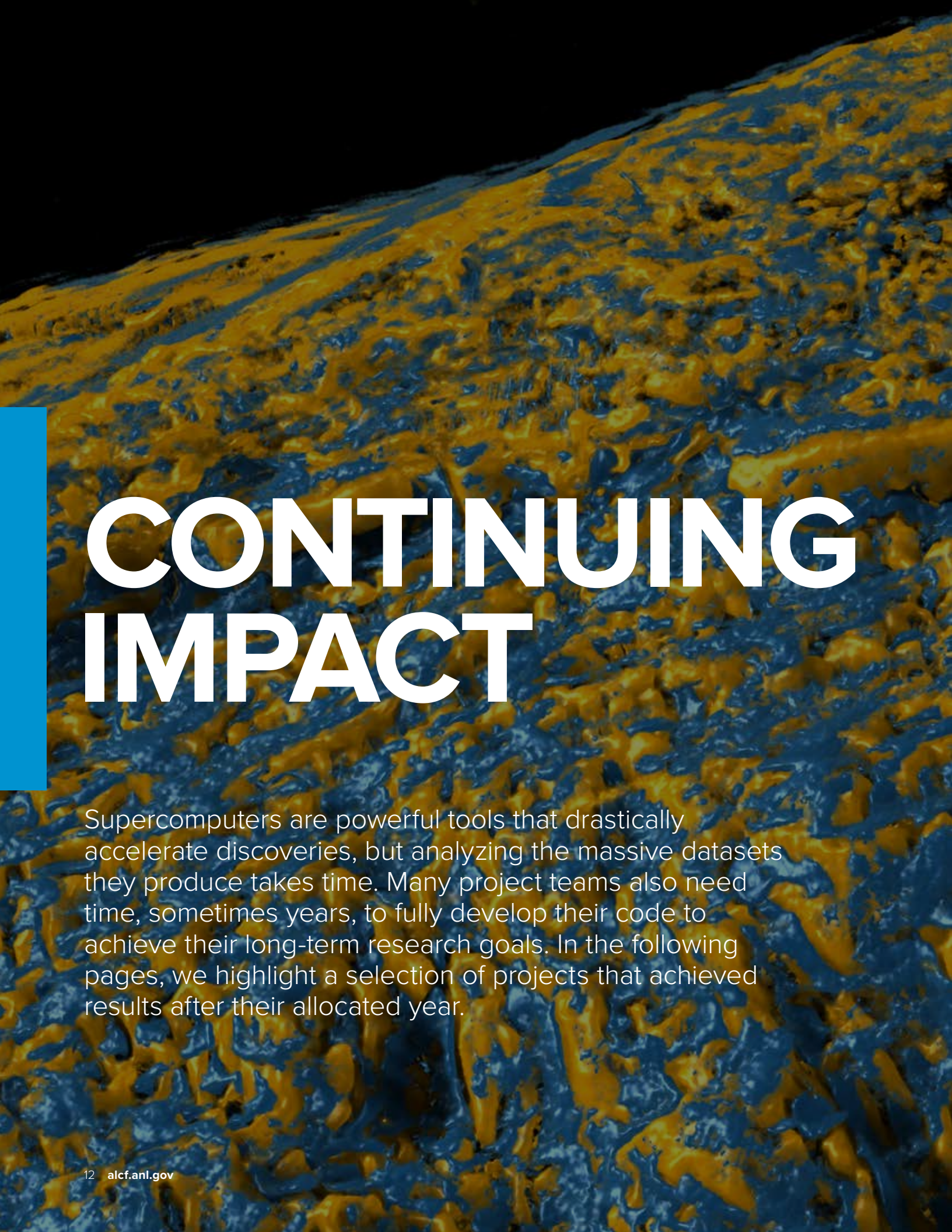
Kenneth E. Jansen
University of Colorado Boulder
Code: PHASTA

The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon

Paul Mackenzie
Fermilab
Codes: MILC, CPS

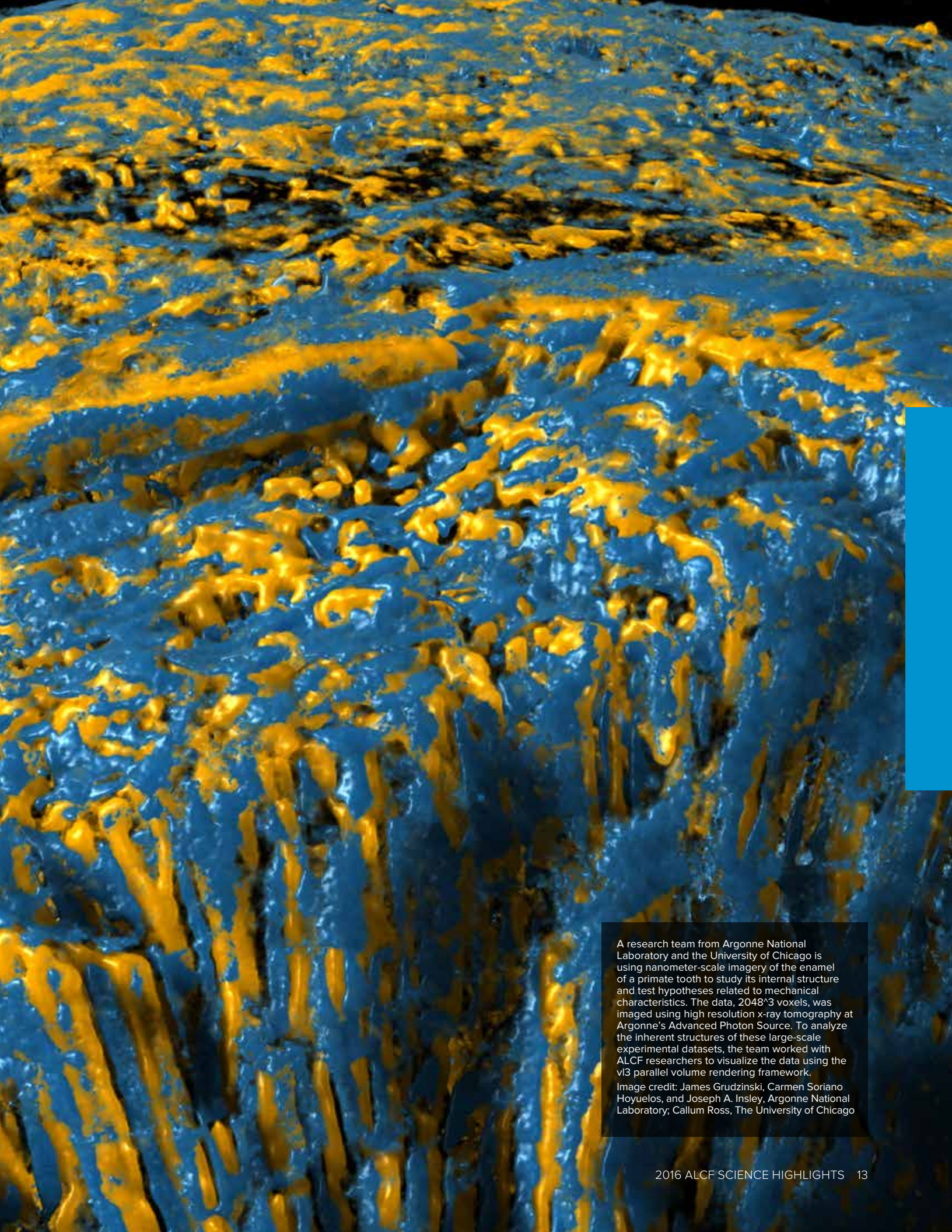
Quantum Monte Carlo Calculations in Nuclear Theory

Steven Pieper
Argonne National Laboratory
Code: GFMC



CONTINUING IMPACT

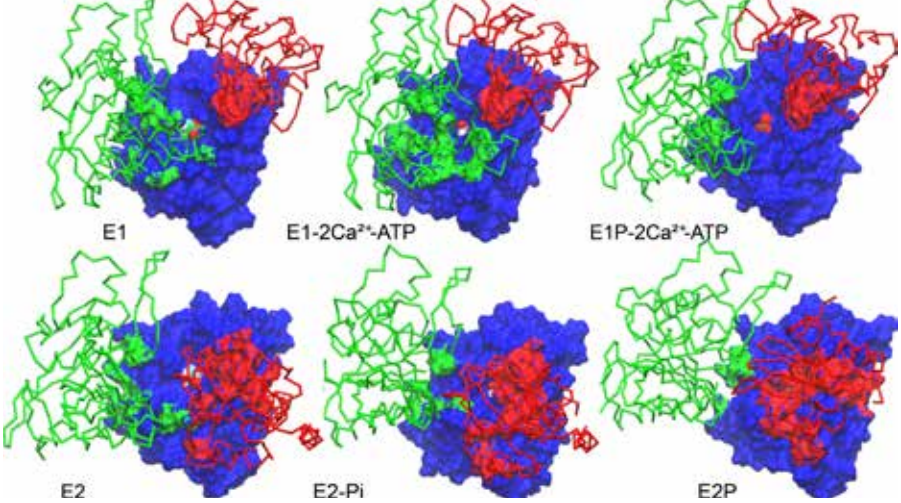
Supercomputers are powerful tools that drastically accelerate discoveries, but analyzing the massive datasets they produce takes time. Many project teams also need time, sometimes years, to fully develop their code to achieve their long-term research goals. In the following pages, we highlight a selection of projects that achieved results after their allocated year.



A research team from Argonne National Laboratory and the University of Chicago is using nanometer-scale imagery of the enamel of a primate tooth to study its internal structure and test hypotheses related to mechanical characteristics. The data, 2048^3 voxels, was imaged using high resolution x-ray tomography at Argonne's Advanced Photon Source. To analyze the inherent structures of these large-scale experimental datasets, the team worked with ALCF researchers to visualize the data using the vl3 parallel volume rendering framework.

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

INCITE
120 Million Core-Hours
Biological Sciences



STUDIES OF LARGE **CONFORMATIONAL CHANGES IN BIOMOLECULAR MACHINES**

BENOÎT ROUX

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The University of Chicago/
Argonne National Laboratory

Image Interaction of cytoplasmic domains in the calcium pump of sarscoplasmic reticulum. These six states have been structurally characterized and represent important intermediates along the reaction cycle. The blue domain, shown in surface representation, is called the phosphorylation domain (P). The red and green domains, shown as Ca traces, are called actuator (A) and nucleotide binding (N) domains, respectively. The red and green patches in the P domain are interacting with residues in A and N domains, respectively. Two residues are considered to be in contact if at least one pair of non-hydrogen atoms is within 4 Å of each other.

Image credit: Avisek Das, The University of Chicago

It is known that malfunctioning proteins can result in a host of diseases, but pinpointing when and how a malfunction occurs is a significant challenge. Very few functional states of molecular machines are determined by experimentalists working in wet laboratories. Therefore, more structure-function information is needed to develop an understanding of disease processes and to design novel therapeutic agents.

Computers have already changed the landscape of biology in considerable ways; modeling and simulation tools are routinely used to fill in knowledge gaps from experiments, helping design and define research studies. Supercomputing provides a window into something else entirely—the ability to calculate all the interactions occurring between the atoms and molecules in a biomolecular system, such as a molecular machine, and to visualize the motion that emerges.

Over the past decade, a University of Chicago team has been developing new computational approaches to simulate virtual models of biomolecular systems with unprecedented accuracy. The team recently concluded a three-year INCITE project to understand how P-type ATPase ion pumps—an important class of membrane transport proteins—operate. In a major breakthrough, they described in atomic detail the complete transport cycle of a large calcium pump called sarco/endoplasmic reticulum calcium ATPase, or SERCA, which plays an important role in normal muscle contraction.

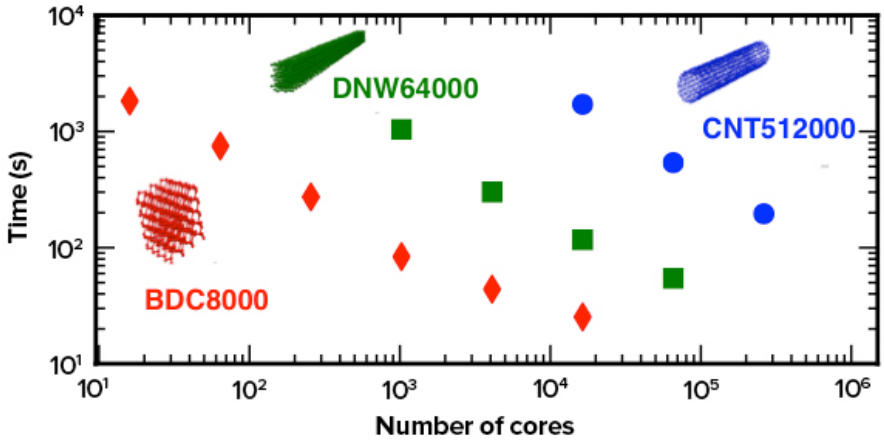
The team used NAMD, a premier molecular dynamics (MD) simulation code that combines two advanced algorithms—the swarm-of-trajectory string method and multidimensional umbrella sampling. NAMD is based on the Charm++ parallel programming system and runtime library, which provides infrastructure for implementing highly scalable parallel applications. When combined with a machine-specific communication library, the string method can achieve extreme scalability on leadership-class supercomputers. ALCF provided maintenance and support for NAMD and helped coordinate and monitor the jobs on Mira.

IMPACT Results from this project will serve as a roadmap for simulating and visualizing the basic mechanisms of biomolecular systems going forward. By studying experimentally well-characterized systems of increasing size and complexity within a unified theoretical framework, this approach offers a new route for addressing fundamental biological questions.

DIRECTOR'S DISCRETIONARY

2.1 Million Core-Hours

Chemistry



SHIFT-AND-INVERT **PARALLEL SPECTRAL TRANSFORMATION EIGENSOLVER**

MURAT KEÇELI

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Argonne National Laboratory

ALBERT F. WAGNER

wagner@anl.gov

Argonne National Laboratory

Image Strong scaling plot of the calculation time needed to get the eigensolution in carbon nanostructures simulations using SIPs and tight-binding density functional theory.

Image credit: Murat Keçeli, Argonne National Laboratory

Synthesis is all about breaking and forming chemical bonds, which result when two different atoms share their electrons. Electrons can only be reliably described by quantum mechanics, which can determine their energies (characterized by eigenvalues) and their spatial distribution (characterized by eigenvectors). The numerical solution of the eigenproblem is generally the most time-consuming part of computing synthesis mechanisms.

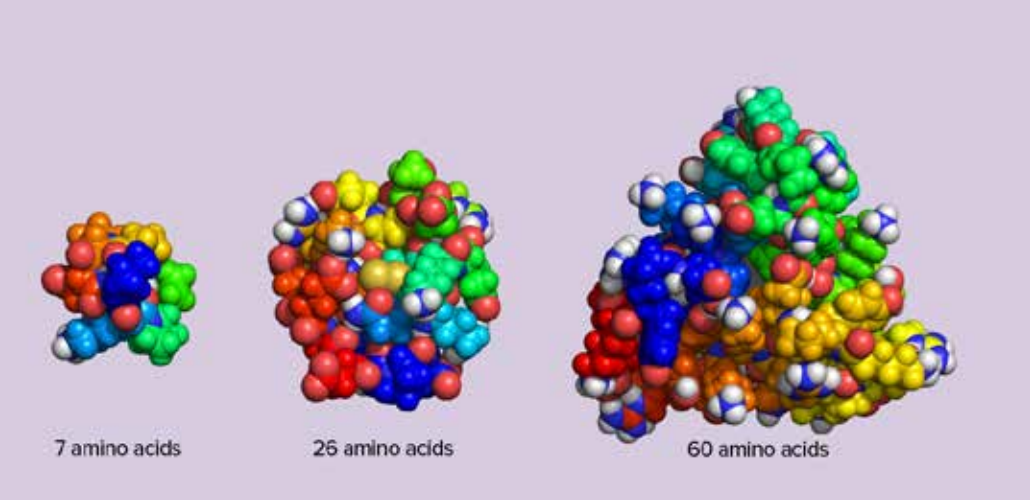
Finding the solution to an eigenproblem for tens to tens of thousands of atoms rapidly escalates to millions of variables and equations that can only be handled by the power of a supercomputer. For this Director's Discretionary project, researchers from Argonne National Laboratory used ALCF resources to test the robustness and scaling capability of their approach for solving the eigenproblem for reduced-scale electronic structure methods applied to large systems.

The approach, Shift-and-Invert Parallel Spectral Transformation (SIPs), was initially developed at Argonne in 2007 to efficiently solve the eigenproblem and thereby obtain the eigenvalues and eigenvectors. The research team optimized the method for massively parallel architectures and specifically enabled density-functional based tight-binding (DFTB) calculations for systems with more than 100,000 atoms utilizing more than 200,000 cores. (DFTB is an approach that can produce useful molecular structures and energetics at a significantly reduced computational cost.)

ALCF helped to port and interface the code with quantum chemistry packages; provided advice on eigensolver algorithms; and assisted with the performance tools used to scale the codes on Mira. The project demonstrated that SIPs could scale beyond 200,000 Blue Gene/Q cores and solve more than 300,000 eigenpairs of a 500,000-by-500,000 matrix in approximately three minutes. Now with the availability of a scalable implementation to diagonalize matrices using a shift-and-invert eigenvalue algorithm, it is possible to simulate hundreds of thousands of atoms using hundreds of thousands of processors, opening the door for significant future research campaigns.

IMPACT The Argonne team is developing methods and software to predict the reaction thermodynamics and kinetics have in synthesis processes. The team's work is expected to enable the discovery and optimization of synthetic approaches to valuable products, such as novel photovoltaic materials, and the inhibition of undesirable products, such as soot arising from combustion.

INCITE
80 Million Core-Hours
Chemistry



TOWARDS BREAKTHROUGHS IN **PROTEIN STRUCTURE CALCULATION AND DESIGN**

DAVID BAKER

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University of Washington

Image The three peptides shown are being experimentally validated by the Baker Laboratory.
Image credit: Vikram Mulligan, University of Washington

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

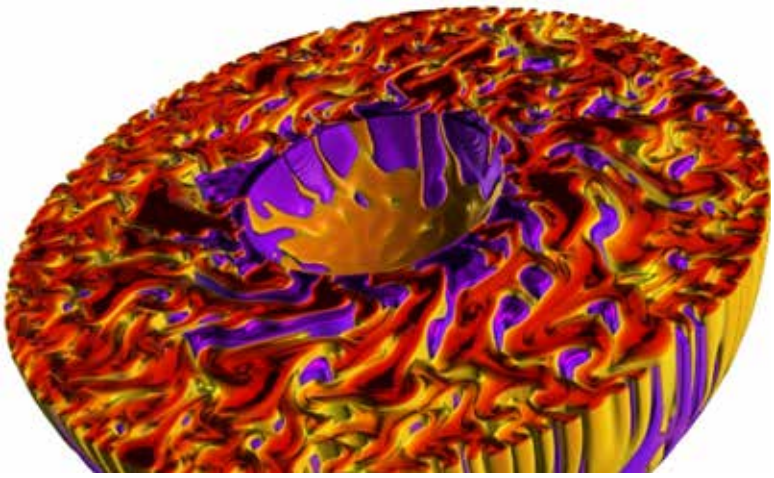
The Rosetta software suite, developed at the University of Washington's Baker Laboratory, is designed to tackle two difficult computational problems: the prediction of protein structure from amino acid sequences and the design of new amino acid sequences to yield a desired function.

To enable the computational design work, the team developed a multistate design approach that allows them to create novel peptides with unique, rigid folds. Their method involves exhaustively enumerating the possible conformations of peptides to search for a sequence that uniquely stabilizes one desired structure and destabilizes alternative structures. The search algorithm benefits enormously from Mira's massively parallel architecture, particularly when assigning each conformational state to a separate core for simultaneous sampling.

The team made fundamental improvements to Rosetta's high-resolution energy function, including its agreement with observational studies and ability to reproduce and discriminate amino acid sequences. They also applied their multistate design approach to develop four diverse examples of folding peptides.

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

INCITE
83 Million Core-Hours
Earth Science



FRONTIERS IN PLANETARY AND STELLAR MAGNETISM THROUGH HIGH-PERFORMANCE COMPUTING

JONATHAN AURNOU

aurnou@gmail.com
University of California, Los Angeles

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

Image credit: Nicholas Featherstone, University of Colorado Boulder

Magnetic fields are generated deep within the interiors of stars and planets through dynamo action, where the motion of a conducting fluid produces an outward flux of heat. As this process remains largely inaccessible to direct observation, researchers aim to leverage high-performance computing tools to develop a new generation of models describing the dynamics at play in the Sun, Earth, and Jupiter.

Solar and terrestrial magnetism, whether generated by iron in the Earth's core or dense plasma at the heart of the Sun, plays an important role in our modern technological society, where Earth's magnetic field shields us from explosive, magnetically driven, solar phenomena.

Through this ongoing investigation, a team of geo- and astrophysicists continue to develop state-of-the-art computational models to describe the interior dynamics of the Sun, Earth, and Jupiter. ALCF staff has participated in application code development of Rayleigh, a pseudo-spectral code designed to study magnetohydrodynamic convection in spheres.

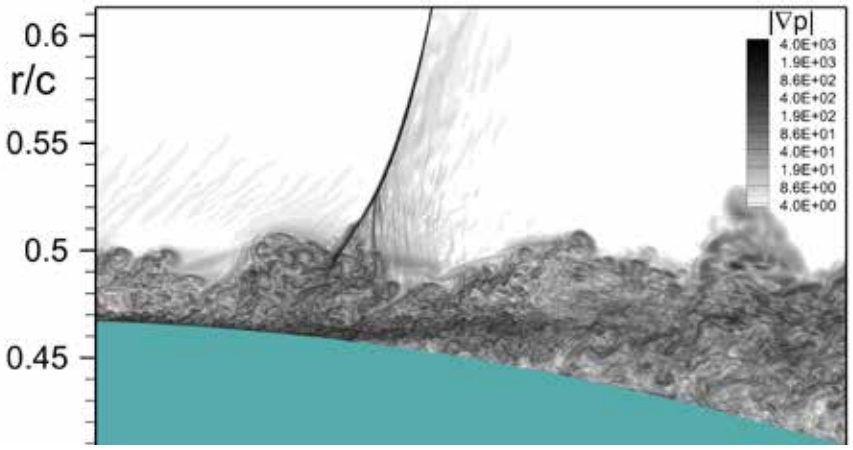
Optimized to Mira, the code has allowed the team to construct high-resolution models detailing how convection transports energy generated by fusion deep within the Sun's core to the solar surface. This code and computer combination can resolve a range of spatial scales previously inaccessible to numerical simulation, ranging from the Sun's diameter to those roughly 1,000 times smaller.

The team also added a new layer to the Rayleigh code, allowing it to solve on radially nested Chebyshev grids, which facilitates both higher accuracy and lower computational cost.

While solar simulations have evolved to include the effects of rotation on kinetic-energy scaling laws, simulations on Jovian dynamics were begun in earnest. The team conducted its first survey to understand the appropriate internal heating functions for Jupiter simulations in preparation for primary, non-magnetic runs, which will constitute the highest-resolution Jupiter simulations yet run.

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

INCITE
135 Million Core-Hours
Engineering



LARGE-EDDY SIMULATION OF THE **BACHALO-JOHNSON FLOW, WITH SHOCK-INDUCED SEPARATION**

PHILIPPE SPALART

philippe.r.spalart@boeing.com
Boeing

Image Contours of the magnitude of the gradient of pressure in the direct numerical simulation, exhibiting the shock wave, turbulence, and separation.

Image credit: Philippe Spalart, Boeing; Kirill Belyaev, Andrey Garbaruk, Michael Shur, Michael Strelets, and Andrey Travin, St. Petersburg State Polytechnical University/New Technologies and Services, Ltd.

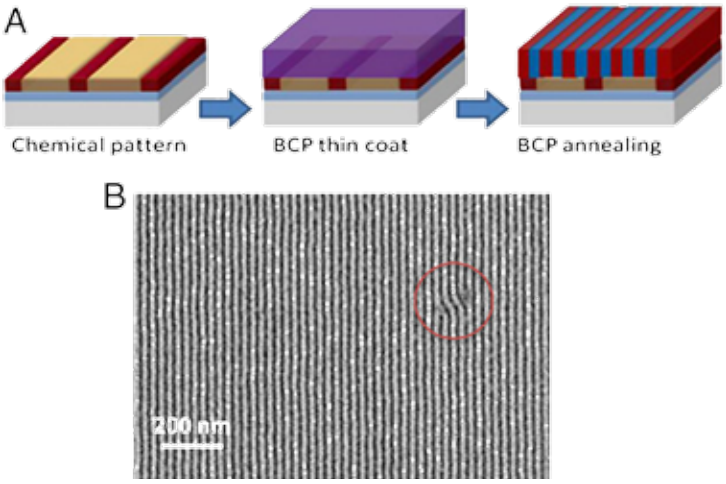
In 1981, NASA researchers (D.A. Johnson and W.D. Bachalo) performed an experiment in which a turbulent boundary layer interacts with a shock wave—a phenomenon that is crucial to the performance of aircraft wings. The experiment has become a widely used test case for computational fluid dynamics and Reynolds-averaged Navier-Stokes (RANS) turbulence models, but it yielded much less information than what a simulation can provide. To contribute valuable data to the worldwide effort to improve turbulence models, researchers from Boeing and St. Petersburg State Polytechnical University set out to perform the first highly resolved simulations of the NASA experiment.

With access to Mira, the team was able to carry out large-eddy simulations of the experiment's axisymmetric transonic flow at the correct Mach (M=0.875) and Reynolds (Re/m=13.6×106) numbers. The team employed a hybrid RANS-improved delayed detached-eddy simulation (IDDES) method, which has no adjustable parameters to match a specific flow other than grid resolution, making grid refinement a necessary element. The IDDES results then prompted the team to conduct an embedded direct numerical simulation (DNS).

Simulations on three progressively refined grids demonstrated improvements in resolving the turbulence with each increase in grid resolution, while the mean flow predicted by the simulation on the finest grid was virtually grid-independent. At the same time, their findings revealed a disagreement of this prediction with the experimental data, particularly on the shock location and post-shock pressure level. In contrast, the agreement for velocity profiles and Reynolds stresses was quite good. The team found that the DNS results were far superior to the IDDES results, even though the DNS domain was relatively narrow and short.

Additionally, the relative failure of IDDES with this flow uncovered a potential issue with the method. While wall-modeled large-eddy simulations, such as IDDES, are considered highly promising for future treatments of turbulence in similar flows, the team's results revealed a need to determine the grid resolution that will enable consistently accurate results in complex flows.

IMPACT Findings from this project will contribute to ongoing efforts to improve turbulence models and enhance the understanding of complex turbulent flows. Improved turbulence models are of great interest to many engineering applications, including the design of aircrafts and gas turbines.



INCITE
60 Million Core-Hours
Materials Science

MOLECULAR ENGINEERING **THROUGH FREE ENERGY MAPPING**

JUAN de PABLO

depablo@uchicago.edu
The University of Chicago/
Argonne National Laboratory

Image (A) Schematic representation of 3x density multiplication of block copolymers on chemical patterns; (B) experimental scanning electron microscope image of a directed self-assembly structure after thermal annealing showing an isolated defect.

Image credit: Tamar Segal-Peretz, Argonne National Laboratory; Juan J. de Pablo, Paul F. Nealey, and Abelardo Ramírez-Hernández, The University of Chicago/Argonne National Laboratory and; Su-Mi Hura, The University of Chicago, Argonne National Laboratory, and Chonnam National University; Vikram Thapar, Cornell University; Marcus Müller, Georg-August-Universität; Weihua Lie, Georg-August-Universität and Fudan University; and Gurdaman Khaira and Paulina A. Rincon-Delgadillo, The University of Chicago

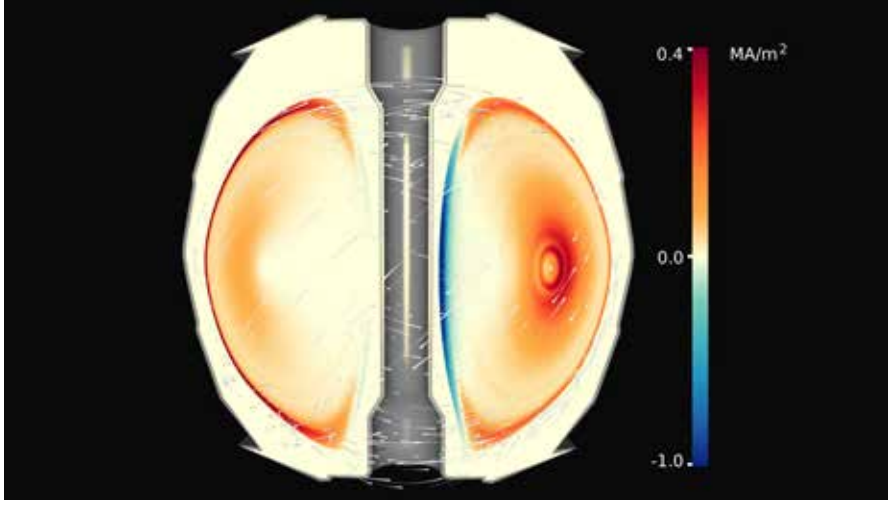
Because traditional transistors and chip technology have reached their limits, next-generation electronic devices will require major advances in miniaturization and fabrication techniques. Self-assembling chains of molecules called block copolymers have favorable length scales, sizes and shapes for being manipulated with simple processing techniques, which makes them attractive for the nanocircuits used on semiconductor devices. However, circuits built at the nanoscale must be near-perfect with very thin and highly dense patterns. To address this critical design challenge, researchers from Argonne National Laboratory and the University of Chicago used Mira to investigate how to avoid defects that arise during fabrication.

To achieve this high level of precision, researchers conducted sophisticated simulations on Mira to identify the key molecular pathways and stable, low-energy states that eliminate defects. The team was able to predict the paths molecules must follow to find defect-free states through large-scale molecular dynamics (MD) simulations based on string method, which is designed to intelligently sample complex conformations through a large number of concurrent replicas.

Only a leadership-class system like Mira can provide massively distributed resources for the concurrent replicas generated by the team's computational model. ALCF computational scientists and staff provided maintenance and support for the MD software GROMACS and LAMMPS, and assisted in coordinating and monitoring production jobs. Results from this project, including a molecular model and energetic mechanism provided at an unprecedented level of detail, were published in the *Proceedings of the National Academy of Sciences* in 2015.

IMPACT These findings will help eliminate defects in next-generation electronic circuits that rely on self-assembling block copolymers by providing key molecular pathways that lead to stable, low-energy states. For industry fabrication, results also point to a thermal annealing process that can be scaled down to deliver defect-free nanocircuitry without introducing expensive, new fabrication techniques.

INCITE
270 Million Core-Hours (ALCF: 100M; OLCF: 170M)
Physics



HIGH-FIDELITY SIMULATION OF **TOKAMAK EDGE PLASMA TRANSPORT**

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Image Developed from Mira simulations, this image shows trapped (left cross-section) and passing (right cross-section) electrons carried in the bootstrap current of a tokamak, which is in contrast to the previous understanding that the bootstrap current is carried by passing particles only.

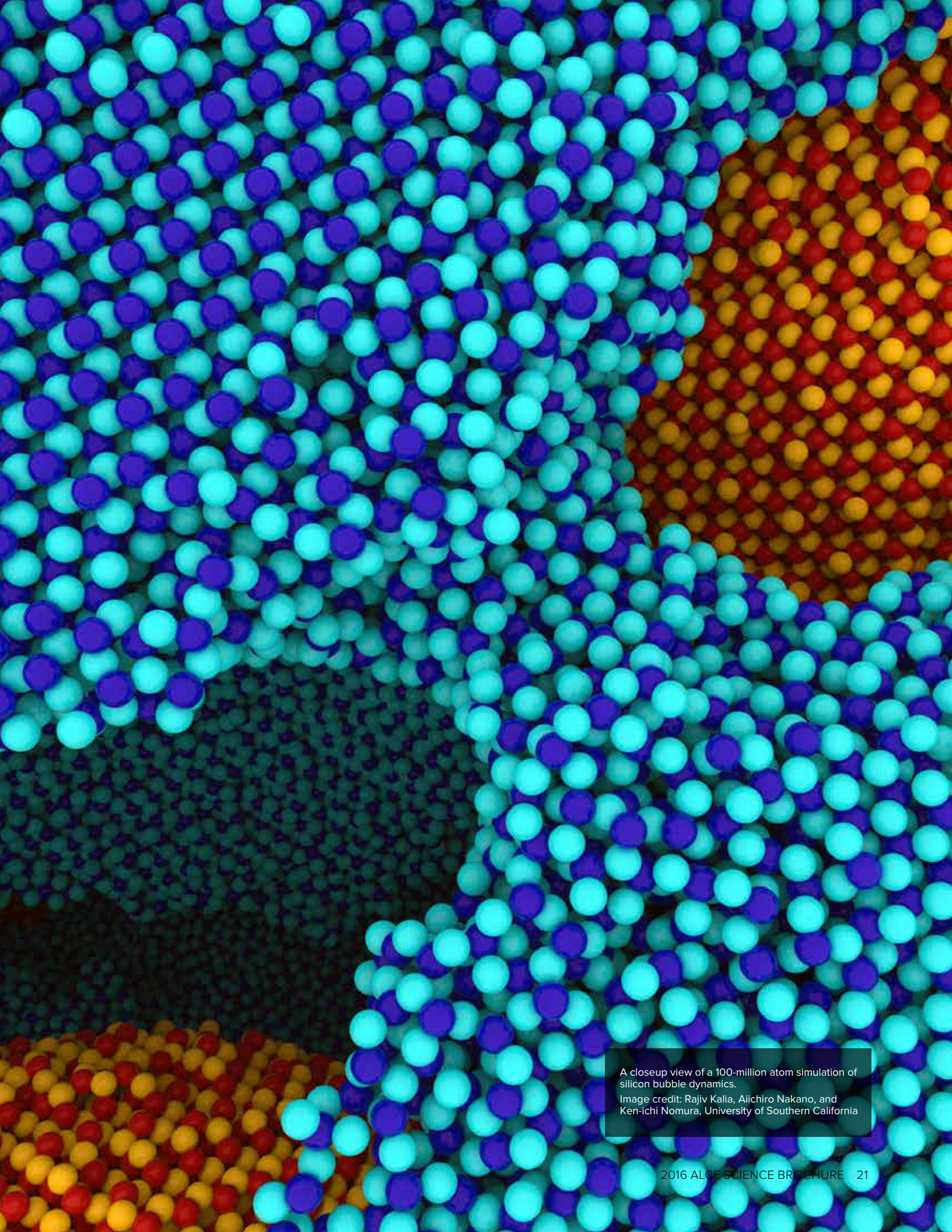
Image credit: Kwan Liu-Ma, University of California, Davis

To develop predictive computational tools for fusion reactors, researchers need to resolve the behavior of plasma across many spatial scales that impact reactor efficiency and plasma stability. Within a tokamak reactor like ITER's, a magnetic field works with a strong electrical current self-generated by the plasma called "bootstrap current" to boost power. Predicting the stability of the bootstrap current is essential because the plasma can collapse if the current is too powerful, potentially damaging vessel walls. One way to improve predictions is to resolve electron behavior in the plasma.

Researchers from Princeton Plasma Physics Laboratory simulated the bootstrap current on Mira using the gyrokinetic code XGC, the only code capable of modeling electron particle behavior from first principles in the whole volume inside the vessel walls in realistic tokamak geometry. Mira's highly parallel architecture and computational power was needed to resolve the multiscale and nonlinear calculations of the electrical current.

In this project, the bootstrap current generated in the plasma of a tokamak fusion reactor was, for the first time, accurately evaluated for realistic, reactor-relevant conditions based on modeled electron behavior. Researchers observed two types of electrons that characterize bootstrap current: passing and trapped. Simulation results showed that, unlike in the core of the tokamak where previous studies have concentrated, trapped electrons mostly carry the current in the edge. With these results, researchers modified a formula that is used to predict the behavior of the bootstrap current. They estimate they reduced the formula's standard deviation from 25 percent to 5 percent, a notable improvement to the predictive accuracy of fusion plasma models.

IMPACT Fusion energy could be a safe and abundant source of power if it proves to work in commercial-scale experimental reactors. With a more precise formula for predicting the behavior of electrical current generated in the plasma of a fusion reactor, researchers can better predict the efficiency of experimental reactors like ITER and plan for future experimental operations.

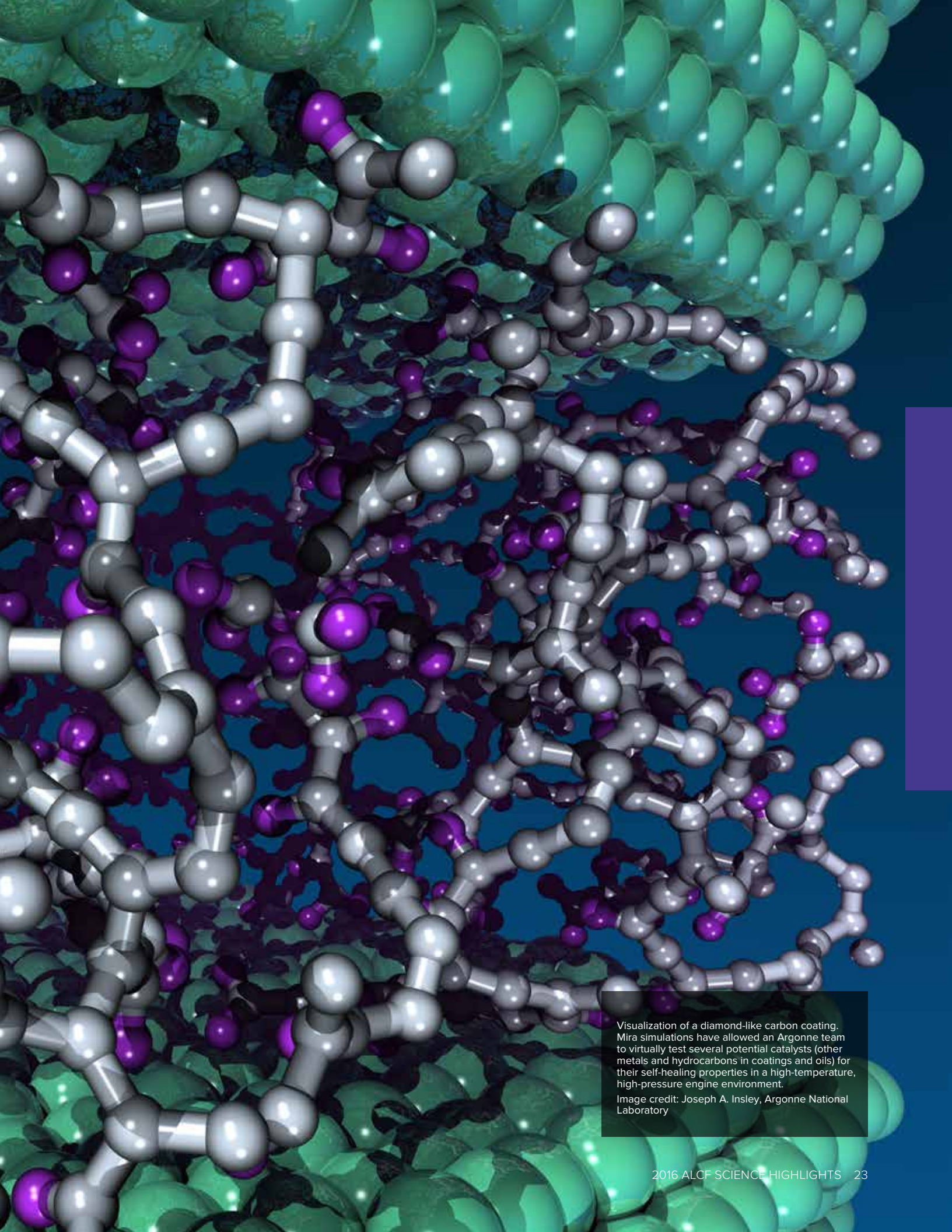


A closeup view of a 100-million atom simulation of silicon bubble dynamics.

Image credit: Rajiv Kalia, Aiichiro Nakano, and Ken-ichi Nomura, University of Southern California

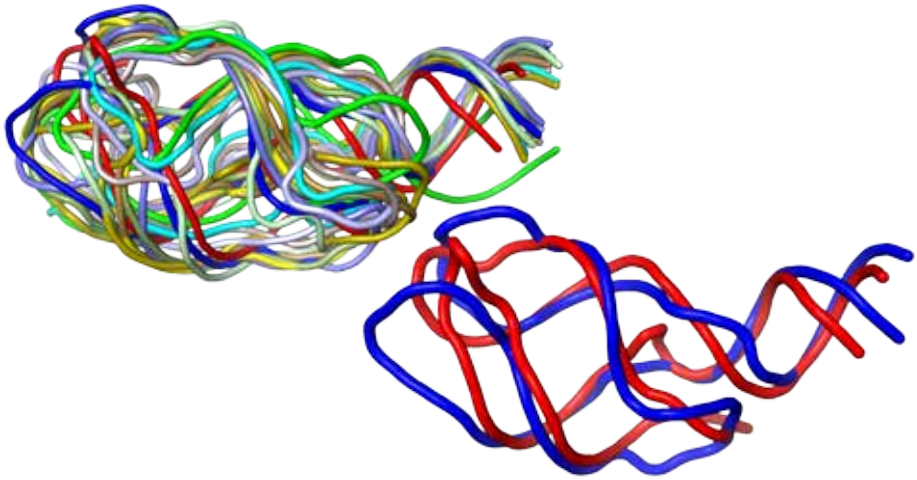
2016 SCIENCE HIGHLIGHTS

The ALCF is accelerating scientific discoveries in many disciplines, ranging from chemistry and engineering to physics and materials science. In the following pages, we highlight a selection of current projects that have produced notable achievements.



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

Image credit: Joseph A. Insley, Argonne National Laboratory



DIRECTOR'S DISCRETIONARY

15 Million Core-Hours
Biological Sciences

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

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Image Explicit 3D structures of adenine riboswitch RNA (PDB ID 1Y26) calculated using RS3D program. Image credit: Wei Jiang, Argonne National Laboratory; Yuba Bhandari and Yun-Xing Wang, National Cancer Institute

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

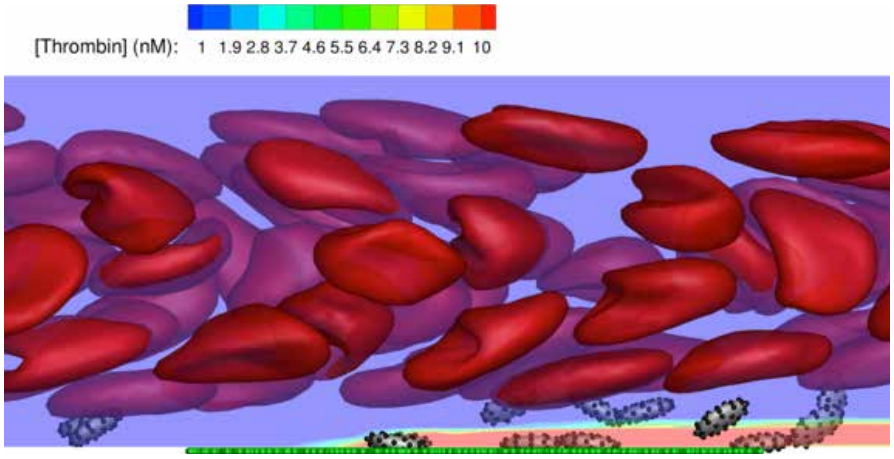
APPROACH The research team developed a robust algorithm and computational program called RS3D to calculate 3D structures of RNA using small-angle x-ray scattering (SAXS) data and known secondary structures as input. Starting from a glob model at nucleotide level of resolution, the algorithm carries out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

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

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

INCITE

90 Million Core-Hours
(ALCF: 50M; OLCF: 40M)
Biological Sciences



MULTISCALE SIMULATIONS OF **HUMAN PATHOLOGIES**

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Image A snapshot of the DPD simulation showing red blood cells, platelets, von Willebrand Factor ligands, and contours of thrombin concentration from the coagulation cascade.

Image credit: George Karniadakis and Alireza Yazdani, Brown University

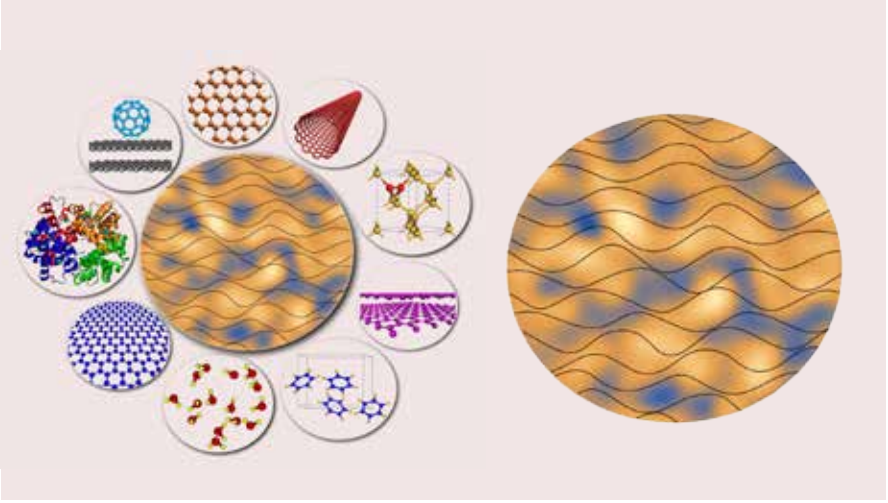
Thoracic aortic aneurysm and dissection (TAAD), a potentially life-threatening condition, occurs when an aneurysm in the aorta expands and tears the artery wall. Due to recent advances in medical imaging and genetics, it has come to light that blood clots, also known as thrombi, play a significant role in aortic dissections. To investigate this further, a Brown University research group is using DOE leadership computing resources to develop the first data-driven, multiscale, multiphysics model of the biomechanics of thrombi in aortic dissection.

APPROACH Leveraging past INCITE awards, the research team has developed a flexible approach in which multiple computer codes are integrated to perform truly multiscale simulations of realistic biological systems. For their current allocation, they are using Mira to develop and test the fractional-order elastodynamics model, the fractal tree closure outflow boundary condition, as well as modeling and validation of platelet aggregation in different geometries and hemodynamic conditions. The team is collaborating with ALCF scientists to optimize I/O, and to develop a pipeline for concurrent simulation and visualization.

RESULTS Researchers have developed numerical methods to address clot formation and platelet aggregation in complex geometries. They have solved the advection-diffusion-reaction (ADR) of different chemical species in the coagulation cascade using the NEKTAR spectral/hp element solver and followed the platelets dynamics based on the force coupling method. The team also developed an approach to solve the ADR equations using the particle-based dissipative particle dynamics (DPD) method. This combination of fluid mechanics, biology, and chemistry concepts, and corresponding simulation codes has allowed them to make significant progress in the modeling of red blood cells in healthy and diseased conditions. Additionally, a multiscale framework has been developed to couple these heterogeneous continuum and atomistic solvers to address the challenging multiscale problems, especially those in pathological conditions, such as TAAD.

IMPACT A better understanding of the roles of thrombi in aortic dissection could lead to improved testing and treatments for the disease. Findings from this project will have important implications for a host of other vascular conditions, providing information that could contribute to improved treatments for a broad class of medical problems.

ALCC
175 Million Core-Hours
Chemistry



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

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

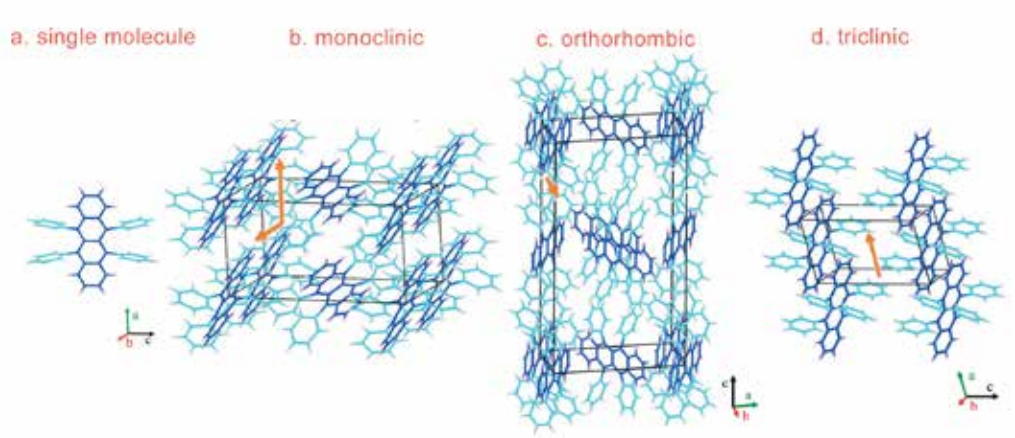
Image credit: Robert A. DiStasio, Cornell University; Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society and University of Luxembourg

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

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

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

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



ALCC
120 Million Core-Hours
(ALCF: 100M; NERSC: 20M)
Materials Science

COMPUTATIONAL DESIGN OF **INTERFACES FOR PHOTOVOLTAICS**

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Image Crystal structure (a), band structure (b), singlet (c), and triplet (d) exciton wave functions of monoclinic rubrene. The weak coupling between molecules produces flat bands. These lead to a charge-transfer like singlet exciton, which may facilitate the transition to two triplet excitons centered on neighboring molecules.
Image credit: Reproduced from *Crystal Engineering Communications,* DOI: 10.1039/c6ce00873a (2016)

The quest for clean, sustainable energy is driving the development of emerging technologies, such as organic photovoltaics and dye-sensitized solar cells. The functionality and efficiency of these devices are often determined by interactions at the interface between two materials. This project is conducting large-scale, massively parallel first-principles quantum mechanical (QM) and molecular dynamics simulations to probe the physical attributes of organic and inorganic interfaces.

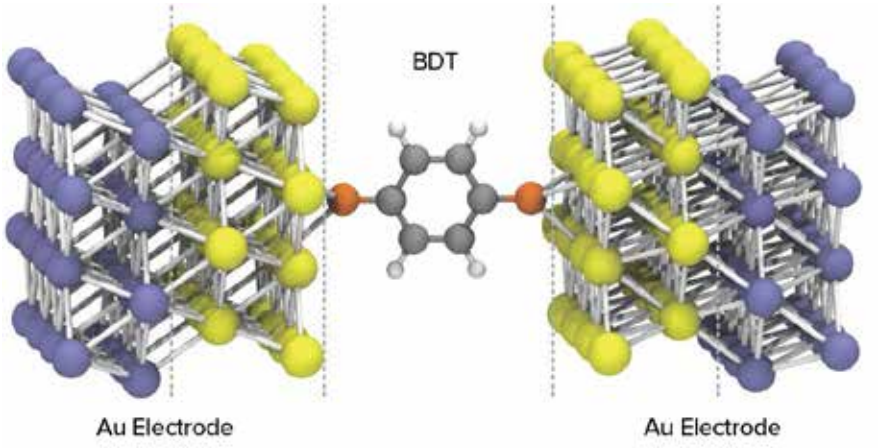
APPROACH Researchers are using the molecular simulation code, FHI-aims, to run fully QM simulations of the structure and electronic properties of the nanostructured functional interfaces found in organic and hybrid solar cells. ALCF was instrumental in helping the team parallelize GAtor, a genetic algorithm for structure prediction and design of molecular crystals.

RESULTS Singlet fission (SF), the conversion of one singlet exciton (opposite-spin electron-hole pair) into two triplet excitons (same-spin electron-hole pairs) with about half the energy, may lead to the realization of high-efficiency organic photovoltaics by generating two carriers from one photon. Recently, SF has been observed in molecular crystals of rubrene, an organic semiconductor known for its high carrier mobility. The team found that the crystal packing of rubrene polymorphs induces significantly different coupling between neighboring molecules, which modifies electronic and excitonic properties. In particular, the weak coupling between molecules in a monoclinic structure produces flat energy bands, which lead to a singlet exciton with an almost pure charge transfer character. This may facilitate the transition to two triplet excitons centered on neighboring molecules. The team expects SF to occur in monoclinic rubrene with a high efficiency, possibly rivalling that of pentacene, the quintessential singlet fission material.

These results demonstrate that the SF efficiency in organic semiconductors may be enhanced by manipulating the crystal packing. Computational modeling may thus provide valuable insight and guide synthesis efforts toward better materials for singlet fission photovoltaics.

IMPACT This research will advance the current state-of-the-art in first-principles simulations and allow researchers to reveal design rules for organic and hybrid materials with desired properties. The theoretical understanding developed in this project will catalyze the emergence of new design paradigms for next-generation solar cell technologies.

ALCC
16 Million Core-Hours
Chemistry



PT-SYMMETRIC QUANTUM MECHANICS FOR REAL-TIME ELECTRON TRANSPORT SIMULATIONS

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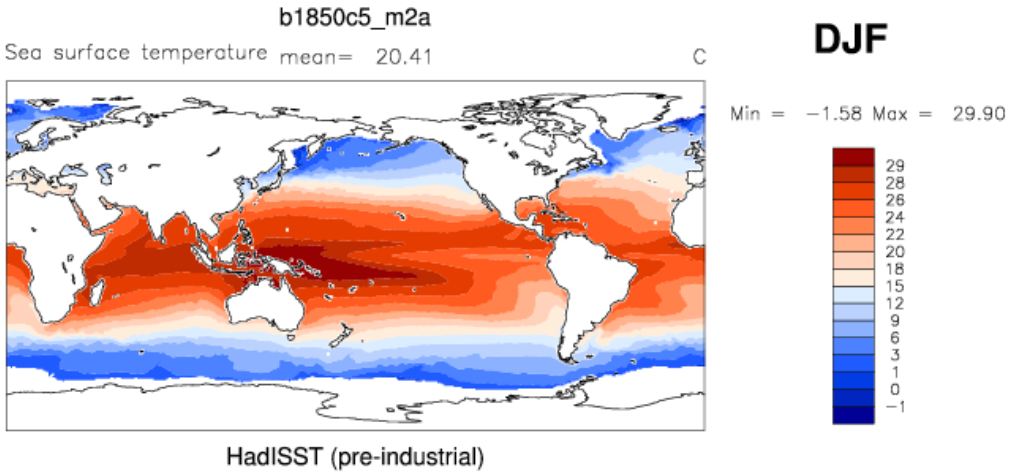
Image A prototypical, single-molecule molecular junction formed by 1,4-benzenedithiol (BDT) and a pair of gold (Au) electrodes.
Image credit: Justin E. Elenewski, George Washington University

For decades, computer manufacturers have been able to double the number of transistors within a given integrated circuit every two years—a phenomenon known as Moore's Law. While this has driven massive growth in computing power, traditional silicon transistor and chip technology is reaching its limit and new technologies must be developed. To identify viable candidate systems for molecular electronics, a team of researchers led by George Washington University is using Mira to develop a theoretical and computational framework for the real-time simulation of electronic transport in nanoscale molecular devices with the ultimate goal of understanding the physics underlying molecular electronics.

APPROACH The team is exploiting the computational power of Mira by expanding CP2K, a massively parallel density functional theory simulation package, to include extensions based on non-Hermitian quantum mechanics. These methods facilitate the simulation of electronic transport in real-time with electrons entering and leaving a system at its boundaries in a manner that mimics actual, open electronic devices. Without Mira, the team would not be able to run efficient simulations of realistic systems, which require scalable and massively distributed resources. To help the team make the most of their computing time, ALCF staff assisted in porting CP2K to Mira's IBM Blue Gene/Q architecture. In doing so, they have parallelized a module designed to calculate the exact exchange-correlation functional with OpenMP and designed a hybrid scripting mode to launch a large number of concurrent CP2K jobs.

RESULTS The team has successfully simplified the mathematical formulation of their method and is extending simulations to 3D nanoscale junctions. They report some of these results and other calculations driven by improved simulation codes in recent papers in *Journal of Physical Chemistry C*, *Physical Chemistry Chemical Physics*, and *Physical Review B*.

IMPACT The results of this study provide a theoretical and computational foundation for the design of next-generation electronic devices, specifically those existing at the single-molecule level. Molecular electronics could significantly increase computing power and circumvent the impending failure of Moore's Law.



INCITE
180 Million Core-Hours
(ALCF: 100M; OLCF: 80M)
Earth Sciences

ACCELERATED CLIMATE MODELING FOR ENERGY

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Image This graph shows December–January–February mean sea surface temperature (SST, °C) averaged over five years, as simulated in the ACME v0 model.

Image credit: Julie McClean, University of California, San Diego

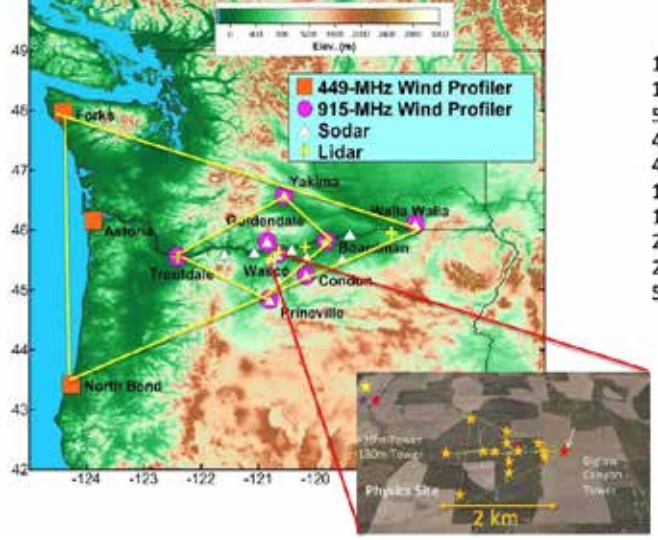
The Accelerated Climate Modeling for Energy (ACME) project is developing a climate and Earth system model that can tackle challenging questions related to the Earth's cryosphere, biogeochemistry, and water cycles. Through ACME, researchers are advancing simulation capabilities to more accurately predict the impacts of climate change, while also preparing for next-generation computing architectures and programming models.

APPROACH Researchers are currently completing high-resolution simulations with the ACME Version 0 (v0) model and will next develop the Version 1 (v1) model. ACME v0 is one of the first high-resolution climate models to be thermodynamically balanced for both the atmosphere energy budget and ocean heat content, and can explicitly resolve oceanic and atmospheric phenomena at tens and hundreds of kilometers, respectively. The enhanced resolution is expected to more realistically simulate the coupled system by reproducing air-sea interactions, eddy-mean flow interactions, tropical storms, and realistic ocean mixing processes. A petascale supercomputer like Mira is required to simulate hundreds of years of climate (approximately 30 million time steps) in a reasonable amount of time. ALCF staff helped improve the performance parallel I/O, vectorization, and threading. They also assisted with the implementation of automated regression testing and the development of the "coupler" (the software that couples the atmosphere, ocean, land, and ice components).

RESULTS The team has completed a 100-year control simulation using pre-industrial climate conditions and an ensemble of present-day simulations approximating climate change from 1970–2010. Team members from several DOE laboratories and the UC San Diego Scripps Institution of Oceanography are comparing the simulation results to satellite and other observational data for quantities like sea surface temperature and precipitation. These results will be used to identify aspects of the Earth system that are well simulated by the high resolution model and where further improvements are needed for the ACME v1 model. The ACME v1 model and associated simulations will be publicly released in late 2017.

IMPACT This project will develop and apply advanced predictive modeling capabilities to investigate the challenges posed by the interactions of climate change and societal energy requirements. The effort will also prepare the research community for a coming paradigm shift in computing architectures and programming models as capability moves toward exascale.

ALCC
15 Million Core-Hours
Earth Science



11 wind profiling radars
17 sodars
5 wind profiling lidars
4 scanning lidars
4 radiometers
10 microbarographs
1 Ceilometer
2 scanning radars
28 sonic anemometers
5 radiative flux systems
& soil moisture

VALIDATION OF RAP/HRRR FOR THE WIND FORECAST IMPROVEMENT PROJECT II

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National Oceanic and Atmospheric Administration

Image Station locations and lists of instruments deployed within the Columbia River Gorge, Columbia River Basin, and surrounding region.
Image credit: James Wilczak, NOAA

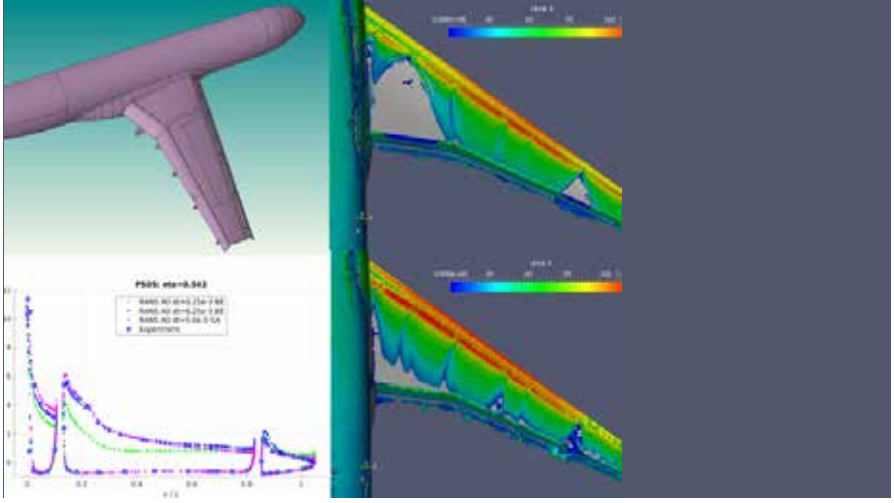
The U.S. Department of Energy aims to increase wind energy from 5 to 20 percent of the nation's total energy use by 2020. This goal can be met by optimizing how wind power is used on the electric grid and making it feasible to introduce wind energy to new regions. Utility operators rely on forecast models like NOAA's 3-kilometer High-Resolution Rapid Refresh (HRRR) to predict how to balance wind energy on the grid with conventional power like coal and nuclear. While HRRR and similar forecast models are effective at predicting wind on flat terrain, they do not have the resolution needed to capture the small-scale wind features that occur in complex terrains, such as mountains, forests, and coastlines.

APPROACH With a combination of new data and computational power, researchers working on the Wind Forecast Improvement Project II are increasing the resolution and improving the physical parameterizations of the HRRR model for more accurate wind predictions in complex terrain. Through March 2017, a wealth of data will be collected in the Columbia River Gorge region along the state borders of Oregon and Washington. Over 15 environmental sensor stations throughout the region are recording wind and weather measurements every 10 minutes for model testing and validation. On Mira, an experimental version of the HRRR with complex terrain-specific enhancements is being evaluated using this observational data.

RESULTS Ultimately, the project will develop a 750-meter resolution model based on the HRRR. By the end of the study, the team will have simulated an entire year of weather forecasts in the Columbia River Gorge region to evaluate how forecasts have improved at the new 750-meter resolution with improved physical parameterizations.

IMPACT In mountainous, coastal, and other complex terrains where wind power could help expand the nation's renewable energy portfolio, a diverse set of small-scale weather features impacts turbine operation and wind power output. Researchers are developing a numerical weather prediction model with a higher resolution and the improved physical parameterizations needed to more accurately predict wind conditions and enable utility operators to plan for integrating wind energy on the grid.

INCITE
70 Million Core-Hours
Engineering



ADAPTIVE DETACHED-EDDY SIMULATION OF A **HIGH LIFT WING WITH ACTIVE FLOW CONTROL**

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University of Colorado Boulder

Image Precisely matched 21 degree angle of attack, high lift wing (with slats and flaps deployed, including supports) wind tunnel model (upper left) produces a highly stalled flow (green data in lower left) when large time steps are used corresponding to wing-fuselage junction separation (upper right image of velocity near the wall) being over-predicted. Smaller time steps capture the unsteady dynamics properly in this region as shown in lower right figure and lower left agreement with experiment.

Image credit: Riccardo Balin and Kenneth E. Jansen, University of Colorado Boulder

With this INCITE award, researchers propose to develop adaptive detached-eddy simulations of synthetic jet active flow control on a multicomponent realistic high lift wing configuration. Researchers will demonstrate that recent developments in parallel adaptive meshing and parallel solver technology can yield fundamental insights into the complicated physics of flow control on real aircraft configurations.

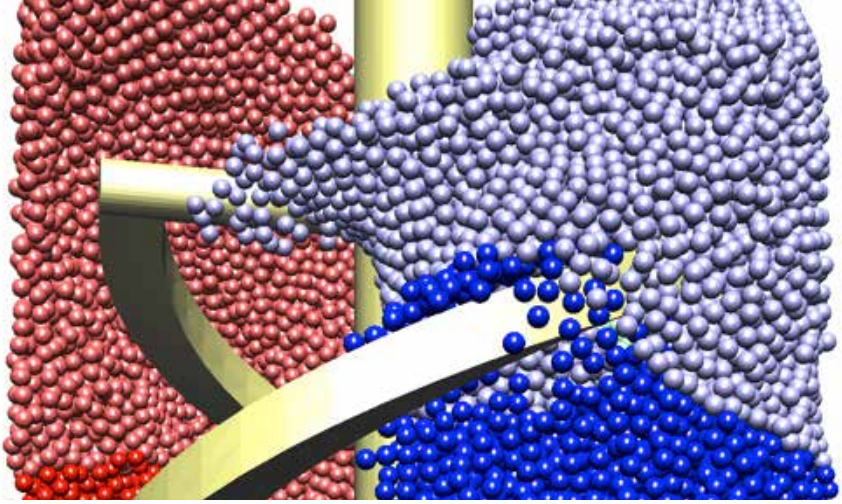
APPROACH The computational approach used for these simulations is the finite-element based flow solver, PHASTA, employed with anisotropic adaptive meshing and partitioning procedures. An excellent match to the active flow control simulations of complex and realistic wing configurations, these tools are applicable to flow problems that involve complicated geometries or complex physics.

The team is modeling an array of synthetic jets that have been vectored to augment the stream-wise momentum near the flap suction peak, where separation is typically observed, to limit flap effectiveness for high-deflection angles and angles of attack. These simulations allow for a fundamental study of flow control on a complex aeronautical control surface.

RESULTS The numerical simulations provide a detailed view of the flow interactions, as well as the insights required to understand and exploit the underlying physical mechanisms related to active flow control. Researchers are using the results to show that the proposed baseline configuration is likely to become a reference for future simulations involving a lower fidelity model, such as Reynolds-averaged Navier-Stokes equations. They hope to demonstrate that the recent developments in parallel adaptive meshing and parallel solver technology can yield fundamental insights into the complicated physics of flow control on real aircraft configurations.

IMPACT The simulations will provide fundamental insight into the interaction between synthetic jets and the main flow on a realistic geometry in aeronautics. By redesigning control surfaces to reduce their size, jet fuel usage can be reduced at a cost-savings of approximately $300 million per year.

ALCC
50 Million Core-Hours
Engineering



COMPUTATIONAL DESIGN OF **NOVEL MULTISCALE CONCRETE RHEOMETERS**

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National Institute of Standards and Technology

Image A snapshot from a simulation of mortar in a double-helix rheometer after approximately 200 degrees of rotation. The suspended spheres are color coded by their initial position in the rheometer. Some sections of the suspended spheres are cut out to reveal the movement of spheres that are close to the rheometer blades.

Image credit: Nicos Martys and Steven G. Satterfield, National Institute of Standards and Technology

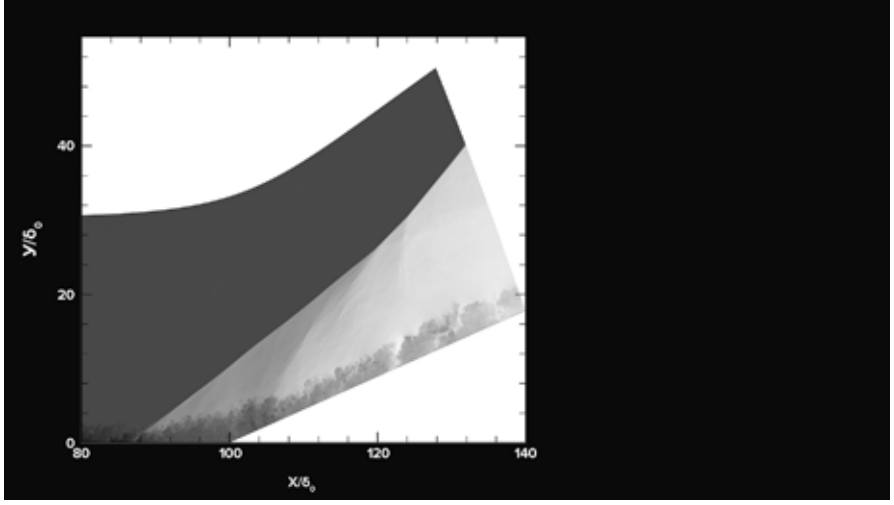
Concrete is the most widely used building material in the world, but the production of its ingredients, namely cement, is a significant contributor to the world's greenhouse gas emissions. The development of more accurate rheometers—instruments used to measure the flow properties of complex fluids—could advance the design of new, more sustainable mixtures of concrete. Researchers from the National Institute of Standards and Technology (NIST) are using ALCF supercomputers to conduct simulations aimed at optimizing the design of rheometer blades to avoid problems of sedimentation, shear induced migration, and other artifacts that impact the physical interpretation of the observed measurements.

APPROACH Due to the complex nature of concrete (a dense suspension comprised of cement, water, and an aggregate), modeling and predicting its flow properties represents a great scientific and computational challenge that requires a large-scale supercomputer like Mira. Building on their work with previous allocations at the ALCF, the NIST research team ran their dense suspension simulator on Mira to continue their efforts to advance the measurement science of concrete and to gain a fundamental understanding of how it flows.

RESULTS The researchers carried out a suite of simulations at a number of different torques to compare fluid flow in several rheometer designs, including four-blade, six-blade, and double-helix geometries. The virtual rheometers were tested with both Newtonian and non-Newtonian fluids. Results from this research are also aiding NIST in the design of Standard Reference Materials for mortar and concrete, which are used by industrial researchers to calibrate rheometers and other measurement instruments.

IMPACT This project is developing the capability to model novel rheometer designs, which will help to guide the manufacturing design and fabrication of rheometers for practical industrial use. Ultimately, this could help researchers zero in on the best new recipes for more sustainable concrete and expand the use of alternative materials. In addition, this work will be useful to other industries that make use of dense, complex suspensions, such as food, pharmaceuticals, and coatings.

INCITE
150 Million Core-Hours
Engineering



DIRECT NUMERICAL SIMULATION OF COMPRESSIBLE, TURBULENT FLOW

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Purdue University

Image Snapshot of the turbulent density field in a separated flow under Mach 2.3 flow conditions, similar to those on the surface of a hypersonic aircraft.

Image credit: Jonathan Poggie, Purdue University

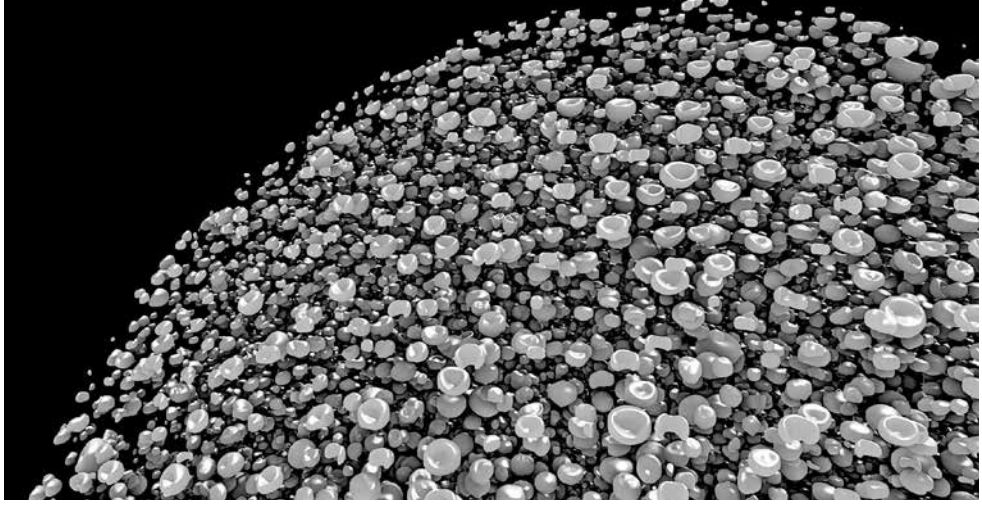
Supersonic flight (above the speed of sound) and hypersonic flight (much faster than sound) are needed to deliver payloads to and from orbit and to develop new military applications and high-speed civilian transportation. When an aerospace vehicle reaches supersonic or hypersonic speeds, turbulent separation of air flow causes intense heating and unsteady mechanical loads. Predicting these damaging conditions is difficult because of the disparity in time scales of large-scale unsteadiness (1–100 milliseconds) and fine-grain turbulence (10–100 nanoseconds). Researchers do not fully understand why large-scale oscillations occur, but they do understand that these frequencies align with the resonant frequencies of aircraft panels, causing severe fatigue loading.

APPROACH Researchers from Purdue University and the Air Force Research Laboratory are investigating supersonic turbulent boundary layers on Mira through massively parallel, direct numerical simulations that use a very large number of grid points. The high-order, finite-difference code HOPS is enabling the team to generate flow separation representative of the boundary layers at the surface of aircraft structures. The main objective is to test the validity of two different models—the amplifier and oscillator models—that describe separation unsteadiness related to pressure fluctuations.

RESULTS The focus of the first year of this two-year project is to study Mach 2.25 separated compression ramp flow. The team has completed a first-year milestone of simulating a turbulent inflow case and is now collecting a large statistical dataset on large-scale separation unsteadiness. The simulations on Mira included three billion cells and scaled to more than 260,000 cores. In future simulations, additional calculations will enable researchers to replicate experimental data and explore the possibility of mitigating aircraft unsteadiness at supersonic and hypersonic speeds with flow control mechanisms.

IMPACT This project is using large-scale direct numerical simulations to test the validity of two different models that describe large-scale unsteadiness in turbulent flow on the surface of aircraft traveling at supersonic or hypersonic speeds. A more precise understanding of turbulent flow will impact the design and operation of these types of aircraft.

INCITE
72 Million Core-Hours
Engineering



DIRECT NUMERICAL SIMULATIONS AND ROBUST PREDICTIONS OF **CLOUD CAVITATION COLLAPSE**

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Image Collapse of spherical cloud with 50,000 bubbles. The generation of microjets directed toward the cloud center causes the formation of cap-like bubble shapes.

Image credit: Computational Science and Engineering Laboratory, ETH Zürich, Switzerland

Cloud cavitation collapse—the evolution of clusters of vapor bubbles in high-pressure flow—is a violent process that generates highly localized, large-amplitude shock waves and microjets. Cavitation collapse is a significant cause of wear in high-pressure injection engines and hydroelectric turbines. New insights into the crucial steps of the collapse process have been obtained by performing simulations at unprecedented resolutions and by exploiting multilevel Monte Carlo methods for robust predictions.

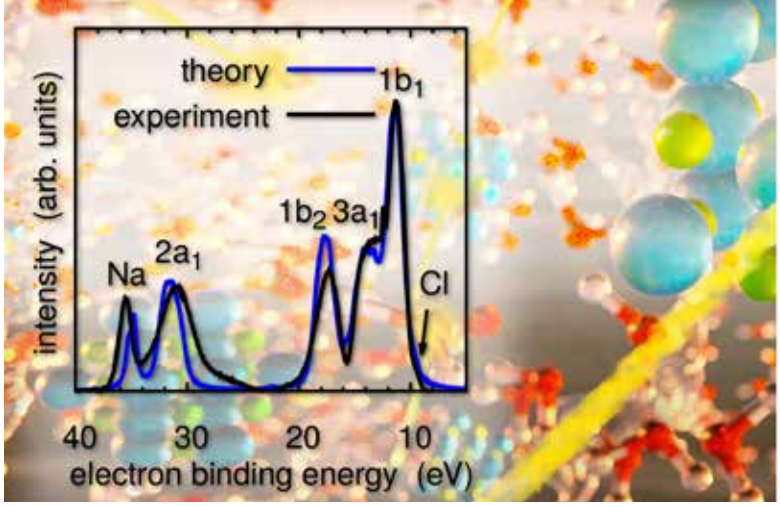
APPROACH Simulation of cloud cavitation collapse requires two-phase flow solvers capable of capturing interactions between multiple deforming bubbles, pressure waves, formation of shocks, and their interactions with boundaries and turbulent vortical flows. For this multiyear INCITE award, researchers from ETH Zürich are using a two-phase compressible flow code, CUBISM-MPCF, to capture the collapse of more than 50,000 bubbles interacting with a complex flow field at unprecedented resolution and performance.

RESULTS In year one of the study, the team used Mira to simulate a free-field collapsing cloud of 50,000 bubbles and a cloud of 20,000 bubbles in a homogenous turbulent flow. The simulation considered different geometrical arrangements (such as spherical or cylindrical), densities, and distributions (random or structured). These studies revealed that cavitation begins with the initiation of collapse at the bubble surface, followed by the formation of center-directed microjets that induce pressure orders of magnitude higher than the ambient pressure.

Now the work is focused on quantifying uncertainties in cloud peak pressures and collapse times under random initial conditions. Simulations of 5,000 to 10,000 bubbles permit 20,000 to 80,000 sources of randomness related to bubble radii, position, and vapor pressure. By exploiting a newly developed multilevel Monte Carlo method, researchers can simulate more sources of randomness than any other statistical sampling approach by up two orders of magnitude. These investigations quantify probable ranges of critical quantities such as the peak pressure.

IMPACT Researchers predict that information gained from these simulations will drastically improve understanding of cloud cavitation collapse in turbulent flows. This INCITE work has already identified steps in the collapse process. The team's work is expected to revolutionize the development of engineering models for the prediction of the cavitation damage potential.

INCITE
150 Million Core-Hours
Materials Science



COMPUTATIONAL SPECTROSCOPY OF **HETEROGENEOUS INTERFACES**

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Image Comparison between experimental and theoretical photoelectron spectra of a solution of sodium chloride in water.

Image credit: Robert Siedel and Bernd Winter, Helmholtz-Zentrum Berlin for Materials and Energy; Alex Gaiduk and Jonathan Skone, The University of Chicago; Giulia Galli and Marco Govoni, The University of Chicago/ Argonne National Laboratory

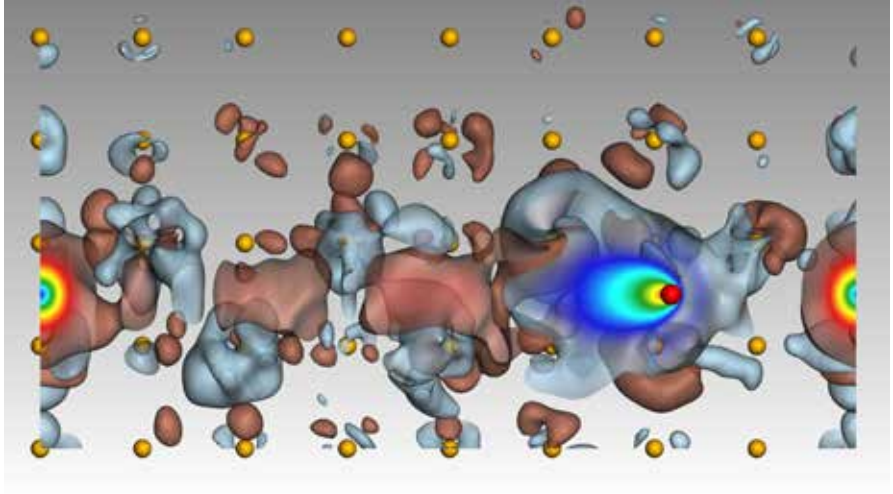
Heterogeneous interfaces between solids, nanoparticles, and liquids play a fundamental role in determining materials properties. With an understanding of the microscopic structure of solid-water and solid-electrolyte interfaces, researchers can better predict the properties of optimal materials for applications, such as water splitting, the production of clean fuels, and energy storage. However, the properties of interfaces are seldom explicitly included in computational models due to the complexity and cost of the associated calculations.

APPROACH With this INCITE project, researchers are developing accurate and efficient computational methods to study heterogeneous interfaces in materials. The team has optimized the Qbox and WEST codes for Mira to enable calculations of opto-electronic (e.g., photoemission and absorption) and vibrational spectra (e.g., sum frequency generation) integrated with large-scale *ab initio* molecular dynamics (AIMD) simulations. This capability, combined with the petascale power of Mira, provides a practical time-to-solution for identifying vibrational signatures of specific reaction pathways that occur at interfaces, and for sampling many configurations from Qbox for input to many-body GW calculations with WEST.

RESULTS The research team conducted a combined computational and experimental study of the photoelectron spectrum of an aqueous solution of sodium chloride. With Mira, they performed first-principles calculations using hybrid functionals and many-body perturbation theory at the G_0W_0 level, starting with wave functions computed in AIMD simulations. The results provided excellent agreement between theory and experiments for the positions of both the solute and solvent excitation energies on an absolute energy scale and for peak intensities. The team recently published their results from this study in the *Journal of the American Chemical Society.*

IMPACT This project is developing open-source computational protocols to enable accurate calculations of the electronic properties of electrolyte solutions and interfaces important to energy-related applications. Theorists and experimentalists alike can use analysis tools derived from the calculations to interpret experiments and to optimize materials properties to improve clean fuel production and solar energy applications. In addition, the work will help establish a strategy to enable the comparison of *ab initio* data with experiments carried out at light sources, such as Argonne's Advanced Photon Source.

INCITE
70 Million Core-Hours
Materials Science



ELECTRONIC RESPONSE TO **PARTICLE RADIATION IN CONDENSED MATTER**

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Image Difference between the time-dependent non-equilibrium electron density and the equilibrium electron density (at t=0) as the projectile proton transverses in gold at the velocity of v=2 atomic units.

Image credit: Liam Krauss, Lawrence Livermore National Laboratory

Researchers from the University of Illinois at Urbana-Champaign and the University of North Carolina at Chapel Hill are investigating the electronic response of semiconductors and DNA to highly energetic particle radiation. Understanding these dynamical phenomena at an atomistic level is central to a wide range of applications, from aerospace electronics to ion-beam technology to proton-beam therapy.

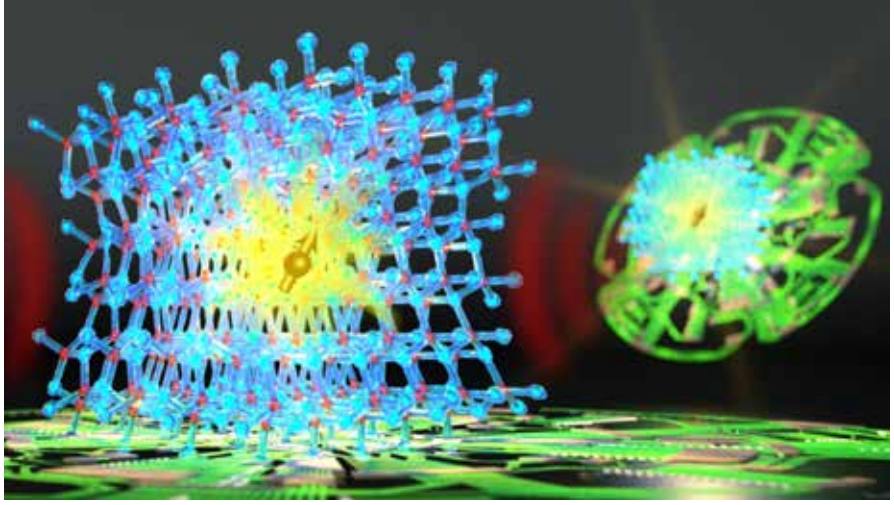
APPROACH A fast, charged particle entering a target material produces complicated effects on a range of length and time scales. At the atomistic level, these begin on atto- to femto-second (one-quintillionth to one-quadrillionth of a second) time scales. Existing mathematical models for calculating the so-called electronic stopping power (rate of energy transfer from the penetrating charged particle to electrons in the target material) lack predictive capability and microscopic details. At the same time, first-principles simulations of non-equilibrium electron dynamics for modeling the energy transfer process are computationally very demanding.

The team's implementation of Ehrenfest molecular dynamics into the Qbox (qb@ll branch), based on real-time time-dependent density functional theory, combines the quantum dynamics of electrons and the classical movement of ions for modeling non-equilibrium dynamics in large complex systems. Together with researchers from Lawrence Livermore National Laboratory, the team focused its code development on strong scalability over many processors, allowing for accurate dynamical simulations of materials that consist of thousands of electrons on these ultrafast time scales.

RESULTS On Mira, the team is modeling electronic stopping processes in technologically important semiconductor materials with different band gaps, or degrees of electrical conductivity, and native defects. Preliminary studies have shown that both of these properties influence electronic stopping significantly. The team is also examining how highly energetic protons transfer their kinetic energy to electrons in DNA and water, as the proton radiation can directly damage DNA or indirectly damage it through ionization of water molecules.

IMPACT This project is establishing a computational framework for predictive modeling of the electronic response of technologically important semiconductor materials and DNA/water to charged-particle radiation. This work will allow researchers to accurately predict the electronic stopping power from first principles and study in detail the underlying energy transfer mechanism in order to tackle highly important challenges in modern materials research.

ALCC
75 Million Core-Hours
Materials Science



FIRST-PRINCIPLES LARGE-SCALE SIMULATIONS OF **INTERFACES FOR ENERGY CONVERSION AND STORAGE**

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Argonne National Laboratory

Image This figure illustrates the spin of a nitrogen vacancy in aluminum nitride designed for quantum bit applications. As part of this ALCC project, the research team published a paper titled "Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies" in *Scientific Reports*.
Image credit: Hosung Seo, The University of Chicago; Giulia Galli and Marco Govoni, The University of Chicago/Argonne National Laboratory

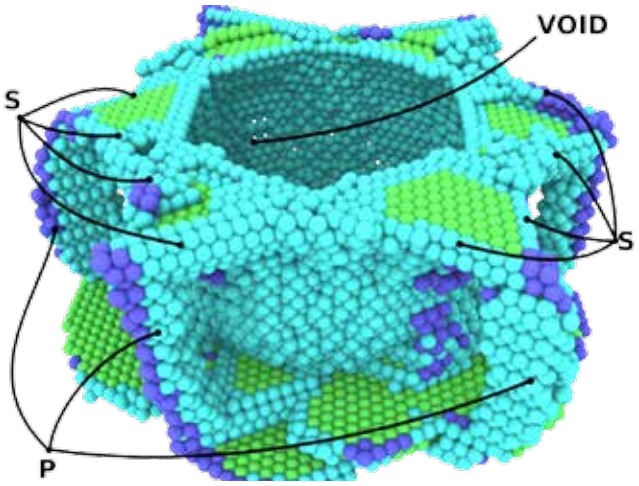
One of the grand challenges in basic energy sciences is to discover new materials that can efficiently extract, convert, and store energy. The design of new quantum materials is also gaining a high level of interest across the scientific community. To support these efforts, researchers are using ALCF resources to develop an open-source code framework that can simulate the electronic properties of large-scale systems. This framework will set the stage for a number of important applications, such as solar-powered fuel production and solid-state quantum computation.

APPROACH The research team has optimized the Qbox and WEST codes on Mira to enable the modeling of microscopic physical and chemical processes occurring at the interface between electrodes and electrolytes and between a defect site and its host material. They are employing *ab initio* molecular dynamics simulations to obtain atomic trajectories, compute ensemble averages, and thermodynamic properties. Many-body perturbation theory methods are subsequently used to compute spectroscopic signatures of solid/liquid interfaces and new potential spin quantum bits in solids.

RESULTS The team published a paper in *Physical Review B*, describing their development of new non-empirical hybrid density functionals with improved accuracy for solids and molecules at a considerably reduced computational cost compared to many-body GW calculations. These results are being used in a combined computational and experimental study of the photoelectron spectrum of prototypical aqueous solutions. In a paper published in *Scientific Reports*, the researchers introduced new strain-driven design schemes to realize defect spin quantum bits for potential applications in quantum computing and sensing. Finally, to enable modeling of perovskites and lead-based nanoparticles, the research team extended the WEST code's functionality with the addition of fully relativistic pseudopotentials. These results, published in the *Journal of Chemical Theory and Computation*, are also available online through open access data collections (www.west-code.org/database).

IMPACT This research is providing the knowledge and computational tools that scientists need to interpret ongoing experiments on fuel production from water, and to establish design rules to predict robust quantum bits in solid state environments. The ability to better predict and design optimized materials will help accelerate the development of advanced energy technologies, and guide future research efforts toward new paradigms for renewable energy and quantum information.

ALCC
20 Million Core-Hours
Materials Science



LARGE-SCALE AB INITIO SIMULATION OF **CRYSTALLINE DEFECTS IN MG-ALLOYS**

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California Institute
of Technology

Image Nanovoid growth in hexagonal close-packed magnesium (Mg). A surprising lack of secondary hardening is evident due to lack of interaction between basal screw (S) and prismatic (P) dislocations.

Image credit: Kaushik Bhattacharya, Michael Ortiz, and Mauricio Ponga, California Institute of Technology

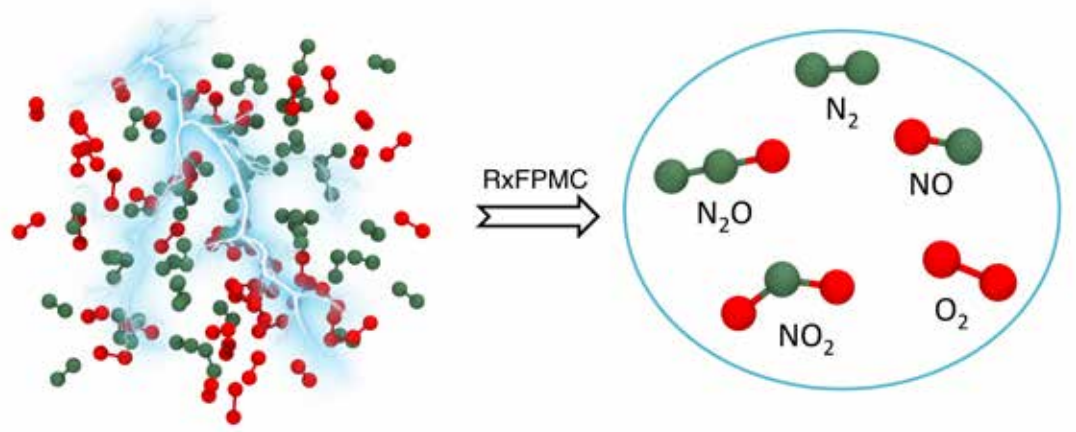
Many important properties of crystalline solids, including metals and insulators, are mediated through defects in the crystal structure. Thus, a predictive understanding of materials properties requires an understanding of these defects. This presents a challenge, as defects intimately couple complex physical and chemical properties and dynamics. This project is pursuing an approach where density functional theory (DFT) is the sole input, and controlled numerical approximations enable the study of defects at realistic concentrations.

APPROACH One of the primary goals of this work is to continue development of MacroDFT, a large-scale code for studying defects in crystalline materials. A research team from Caltech has implemented and assessed the parallel performance of MacroDFT on Mira, demonstrating the accuracy and efficacy of the approach. Already, this has enabled an unprecedented billion-atom DFT computation of selected defects in magnesium that gave rise to new physical insights. And now, utilizing a new coarse-grained framework, they have extended further the capabilities of MacroDFT to the studies of multiple defects, such as dislocations, grain boundaries, etc. Based on the convection of electronic fields according to the deformation gradient of the crystal, this algorithm allows for fast and inexpensive evaluation of the electronic field that can be used *a posteriori* in large calculations.

RESULTS This new algorithm has allowed researchers to obtain new insights into the physics of prismatic dislocation loops in magnesium and has simulated, for the first time, the core of a screw dislocation in magnesium, solely using DFT in a domain large enough to capture the electronic fields. The team used HotQC, a large-scale code for performing coarse-grained simulations of atomic-continuum crystalline systems, to observe nanovoid growth in hexagonal close-packed magnesium, and discovered a surprising lack of secondary hardness.

IMPACT Magnesium alloys have among the highest strength-to-weight ratios and therefore have the potential to revolutionize transport technology. However, due to their low ductility, they have received relatively little attention. But now, an image of exactly how ductility can be manipulated through crystal defects is beginning to emerge through the use of leadership-class computer simulations. Eventually, these studies will lead to a generalized conclusion or model to describe the mechanical behavior of solid-solution materials, and will open an avenue to a more systematic study of alloys.

ALCC
120 Million Core-Hours
Materials Science



PREDICTIVE MODELING OF **FUNCTIONAL NANOPOROUS MATERIALS**

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Image The reactive first-principles Monte Carlo (RxFPMC) approach to efficiently evaluate reaction equilibria was applied to compressed nitrogen-oxygen mixtures under conditions similar to atmospheric lightning strikes.
Image credit: Evgenii O. Fetisov and J. Ilja Siepmann, University of Minnesota

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

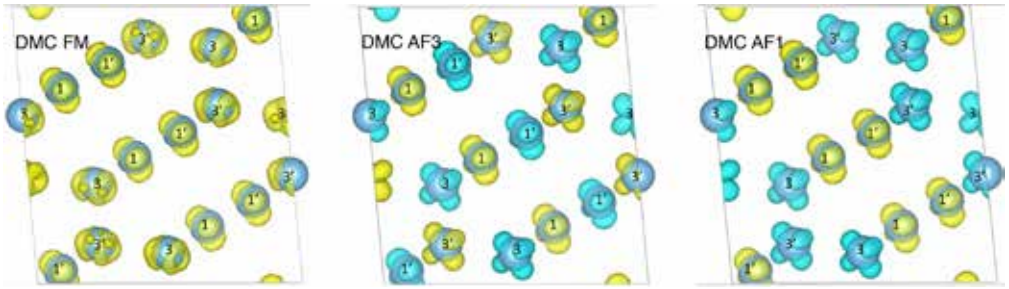
APPROACH Scientists participating in the DOE-funded Nanoporous Materials Genome Center, led by the University of Minnesota, are using Mira to demonstrate and develop a predictive theory and modeling tool that can rapidly screen thousands of materials to pinpoint promising candidates for further research.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

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

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

INCITE

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



QMC SIMULATIONS DATABASE FOR **PREDICTIVE MODELING AND THEORY**

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

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

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

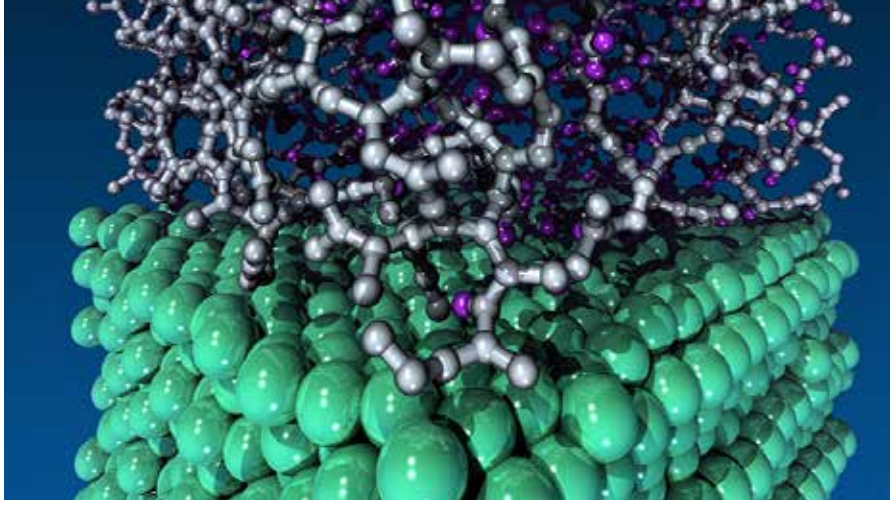
APPROACH Researchers are using the QMCPACK code for a variety of studies, including heterogeneous catalysis of transition metal nanoparticles, magnetic phase transitions, properties of materials under pressure, and strongly correlated materials showing interesting electronic and magnetic properties.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

RESULTS For one study, researchers modeled Ti_4O_7, a titanium oxide that has a range of technological applications due to its complex electronic and magnetic structures. Simulations on Mira have, for the first time, calculated the lowest energy states of Ti_4O_7, revealing its magnetic properties and stable ground state. The team's results were published in *Physical Chemistry Chemical Physics* and will help improve the accuracy of other electronic structure modeling tools, such as the widely used density functional theory.

Additionally, researchers are studying the intermediate concentrations of iron-bearing perovskite and post-perovskite phases of magnesium silicate to better understand the unusual properties observed in the core-mantle boundary layer. Further, they are simulating platinum (Pt) solids, nanoclusters, and surfaces to analyze the surface energies of Pt (111) and Pt (100), which are important in surface and catalytic applications.

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

INCITE
40 Million Core-Hours
Materials Science



REACTIVE MD SIMULATIONS OF **ELECTROCHEMICAL OXIDE INTERFACES AT MESOSCALE**

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Argonne National Laboratory

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

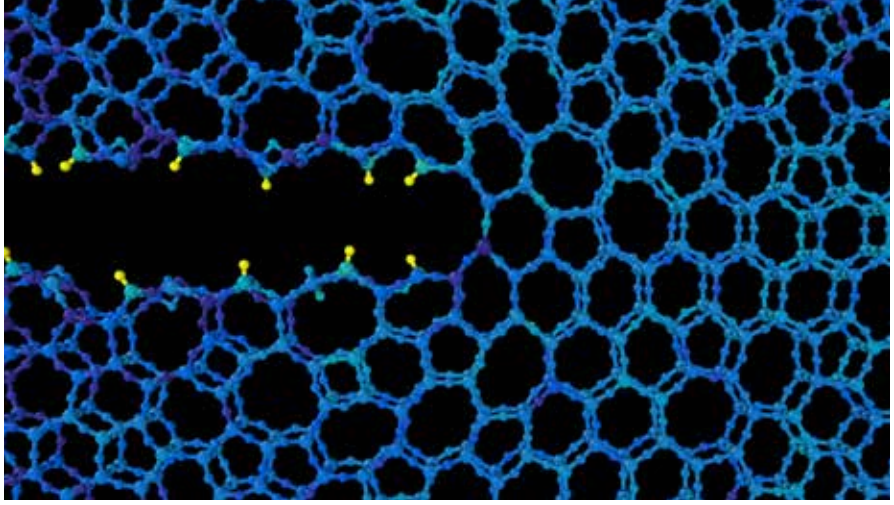
The initial reactions important to chemical bond formation, electron transfer, and other electrochemical processes can occur on the atomistic and molecular scale in a matter of nanoseconds—beyond the detection of many experiments. For the design and development of new materials for energy applications,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

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

RESULTS After tribology experiments showed that a new film was being regenerated at the interface of an engine coating and base oil, researchers turned to Mira to model the underlying reactive processes. The simulations enabled the design of a self-healing, anti-wear coating that dramatically reduces friction and related degradation in engines and moving machinery. With LAMMPS, they modeled as many as two million atoms per simulation, making this one of the few atomistic studies of friction—of any kind, not just tribocatalysis — at this scale. Millions of time steps per simulation enabled researchers to identify the initial catalytic processes that occur within nanoseconds of machine operation. The results of the study were published in *Nature* in 2016, and now researchers are using that discovery to virtually test other potential self-regenerating catalysts.

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

INCITE
126 Million Core-Hours
Materials Science



SiO_2 FRACTURE: CHEMOMECHANICS WITH A MACHINE LEARNING HYBRID QM/MM SCHEME

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Image Crack propagation in a 2D bi-layer of amorphous silicon dioxide modeled with a polarizable interatomic potential. Atoms are colored by their local potential energy on a scale normalized from dark blue, lowest energy, to yellow, highest energy.

Image credit: Marco Caccin and Alessandro De Vita, King's College London; James Kermode, University of Warwick

Understanding the chemo-mechanical phenomena that cause silicates to fracture could prove advantageous to both enabling the process, as in large-scale mining, and eliminating it in products that rely on silicate materials. Researchers are using advanced computing tools to better understand the behaviors that drive stress corrosion and chemically activated crack propagation at both the macro- and microscopic levels.

APPROACH This multiyear INCITE project is pioneering simulation methodologies for predictive modeling of failure processes in oxides using a hybrid quantum mechanical/molecular mechanical (QM/MM) scheme to help describe the fracturing of silicon dioxide in a wet environment.

On the method development side, the team is advancing a novel machine learning approach, Learning on the Fly (LOTF), that significantly reduces the number of expensive QM calculations necessary per unit of simulated system time. This approach dramatically increases the efficiency of ongoing production calculations, reducing the computational cost anticipated for 2016 by approximately 40 percent for the same scientific milestones.

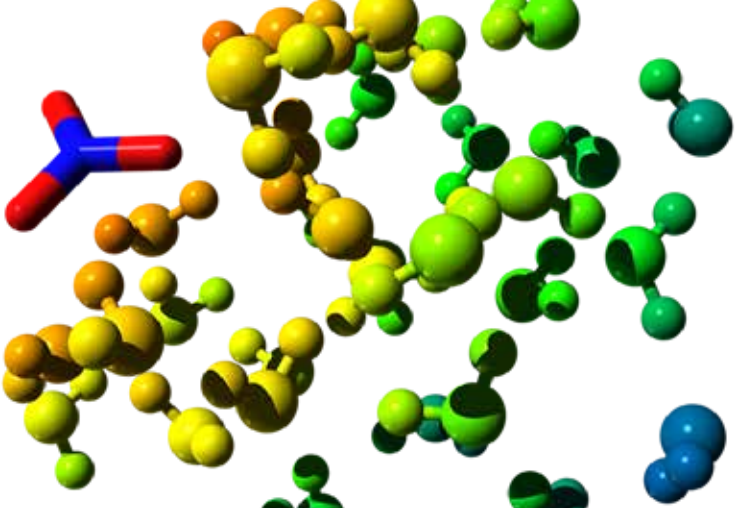
Recently, the group published a paper in *Modelling and Simulation in Materials Science and Engineering*, describing how the LOTF approach can be extended to impurities and defects. This demonstrates the broader impact of the project to develop tools and technology that can be applied beyond silica systems.

RESULTS Simulations have shown 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. Additionally, the completion of production simulations for 2D silica glass systems will help explain the key mechanism underlying stress corrosion cracking and suggest strategies to control it.

Continuing work on machine learning of QM forces is of key importance at this point in the project, as applications in science and machine learning will converge to deliver much larger 3D modeling of silica/water systems.

IMPACT Results from this project have relevance for a broad range of applications in mining, photovoltaics, and biomedical implants. The methodology is also expected to generate fundamental insights that could help rationalize and guide future material designs and novel algorithmic developments.

INCITE
200 Million Core-Hours
Materials Science



STATE-OF-THE-ART **SIMULATIONS OF LIQUID PHENOMENA**

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Iowa State University

Image A nitrate anion (a negatively charged ion) solvated by 32 water molecules in a molecular dynamics simulation.

Image credit: Spencer Pruitt, Argonne National Laboratory

The behaviors of liquids and solutes are critical to understanding many chemical and biological processes, including those that drive energy applications. Ionic liquids are important to the extraction of rare earth elements used in devices like cell phones; and ion solvation, or the diffusion of electrically charged atoms in a solution, is fundamental to our understanding of the natural environment and the development of industrial chemical reactions and energy technologies. Yet, characterizing a solution's complex atomic and molecular interactions in order to optimize its function is a challenge.

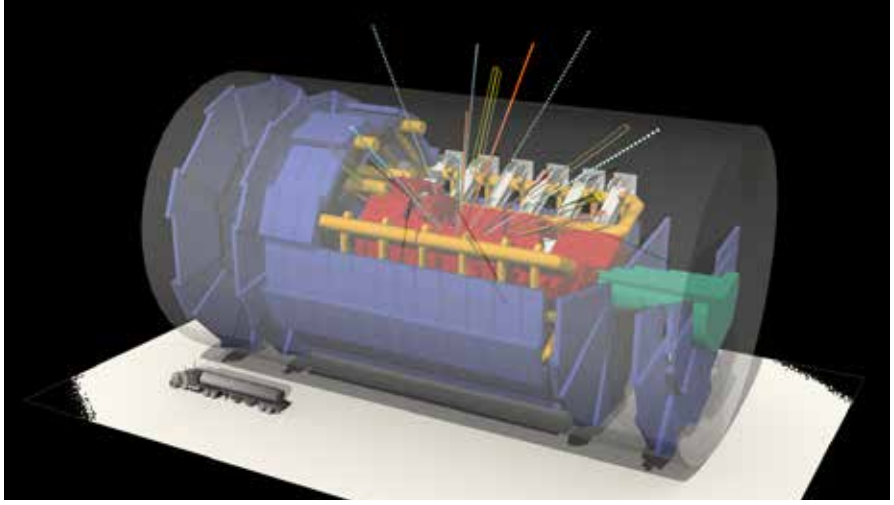
APPROACH Researchers from Iowa State University are executing state-of-the-art dynamical simulations of large ensemble, or "bulk," systems of molecules to obtain predictions of the thermodynamic properties of water and ionic liquids. The simulations are quantum mechanical, based on *ab initio* electronic structure calculations that are capable of modeling subtle quantum effects, which simplified classical models must omit due to computational expense.

Within its quantum chemistry software package GAMESS, the team uses a fragment molecular orbital method to divide the molecular system into smaller units that can be solved quickly and simultaneously on Mira's highly parallel architecture. ALCF staff implemented the multi-level generalized distributed data interface, where multiple instances of a given simulation can be executed simultaneously to speed up the accumulation of statistics for thermodynamic predictions.

RESULTS This project has completed equilibration simulations solving for motion in realistic-sized systems of hundreds of atoms or molecules. Simulations have so far examined the potential of mean force of ionic liquids for rare earth element extraction and the detailed structure of solvation shells around selected ions.

IMPACT Most biological and chemical processes happen in the liquid phase, including the interactions of charged ions in solar cells and batteries and the extraction of rare earth metals from aqueous ionic solutions. This project is simulating the quantum effects that drive water structure and bonding, and ion association in these solutions.

ALCC
78 Million Core-Hours
(ALCF: 62M; NERSC: 16M)
Physics



AN END-STATION FOR INTENSITY AND ENERGY FRONTIER EXPERIMENTS AND CALCULATIONS

THOMAS LECOMPTE

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Argonne National Laboratory

Image An artist's representation of the ATLAS detector at CERN's Large Hadron Collider, showing particles produced in the aftermath of the collision between two high-energy protons (the truck shown in lower left is depicted for scale). Several billion of these kinds of events have been simulated on Mira.

Image credit: Taylor Childers, Joseph A. Insley, and Thomas LeCompte, Argonne National Laboratory

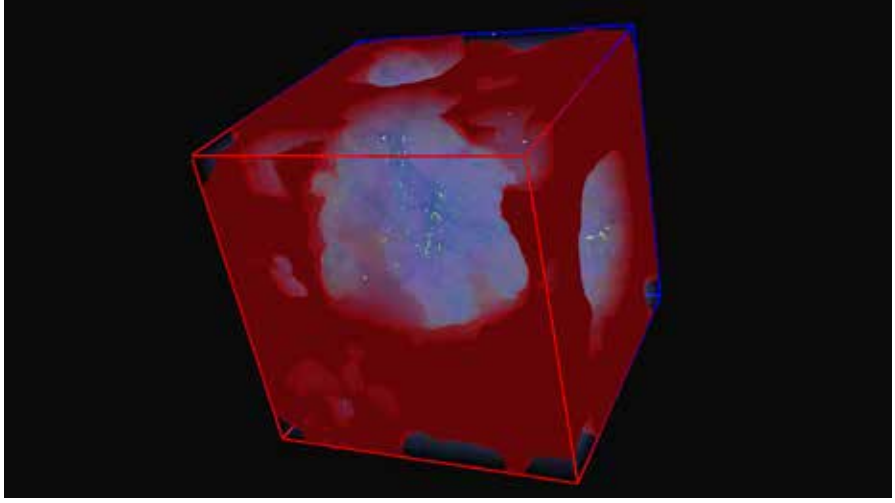
In the field of high-energy physics (HEP), simulating experiments, such as particle collisions at the Large Hadron Collider (LHC), is key to uncovering differences between theory and observation. Subtle deviations from experimental data can lead to discoveries of new physics. Petascale supercomputers like Mira are providing a means to perform increasingly precise simulations as well as calculations that are too intensive for traditional computing resources.

APPROACH Building on a previous ALCC award that focused on simulating LHC events, researchers from Argonne National Laboratory have established an end-station that supports multiple HEP activities with a single allocation. This approach lowers the barriers to entry for scientific communities which have not previously used leadership computing resources, providing a powerful research tool to a variety of HEP projects. Under the previous allocation, ALCF researchers helped the team scale Alpgen, a Monte Carlo-based event generator, to run efficiently on Mira, enabling the simulation of millions of LHC collision events in parallel. The Argonne team continues to work with ALCF staff to optimize and run various HEP codes on the facility's supercomputers.

RESULTS The team continued to perform event generation calculations with Alpgen for LHC's ATLAS experiment. Running these jobs on Mira has allowed the ALTAS community to simulate complex events much more quickly, while freeing the LHC's computing grid to run other jobs. The team also has made strides in scaling and optimizing Sherpa (another event generator used by LHC experiments) and the Adaptive Refinement Tree (ART) code for ALCF computing resources. In addition, the end-station has enabled another Argonne team to use Mira for a series of next-to-next-to-leading order quantum chromodynamics calculations. Thus far, simulations from this ALCC project have led to 25 published papers.

IMPACT This project is showing that supercomputers like Mira can accelerate discoveries for large-scale physics experiments. Running simulations on leadership computing platforms provides three key benefits to the HEP community: increasing the amount of simulated data that can be produced; simulating more complex and realistic events than were previously possible; and helping to evolve a variety of physics codes for emerging platforms, both high-performance and commodity.

INCITE
65 Million Core-Hours
Physics



COSMIC REIONIZATION ON COMPUTERS

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Fermilab

Image Simulation of cosmic reionization. Dark red shows opaque neutral gas, transparent blue is ionized gas, and yellow dots are galaxies.
Image credit: Nickolay Gnedin, Fermilab

Cosmic reionization, the most recent phase transition in the universe's history, is the subject of active research in modern cosmology. But observations from the Atacama Large Millimeter Array and the forthcoming James Webb Space Telescope will make existing theoretical models of reionization obsolete. Hence, the theoretical community is challenged with upgrading simulation technology to a qualitatively higher level to keep theory adequate for comparing with future observations.

APPROACH Taking advantage of advances in supercomputing, the Fermilab research team is carrying out simulations that model all physics relevant to cosmic reionization, using the Adaptive Refinement Tree (ART) code as its main simulation tool on Mira.

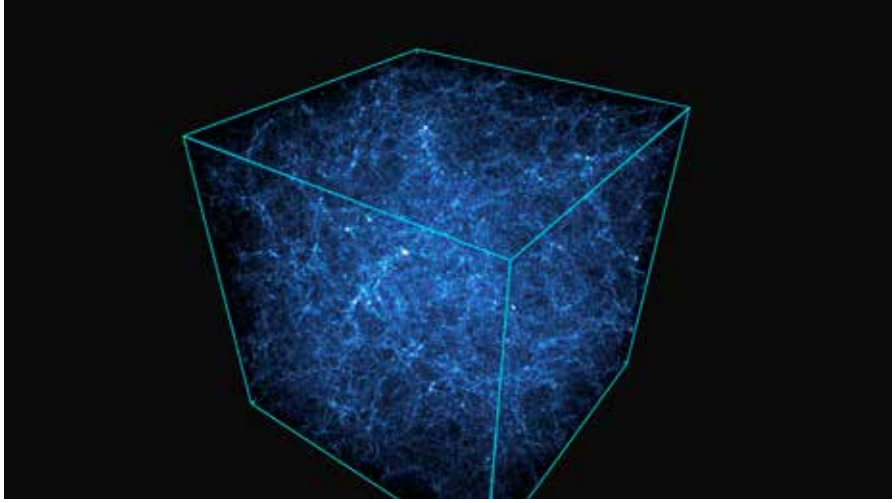
An important objective of this research is to make predictions for future observations of the redshifted 21-centimeter line of neutral hydrogen. That line, coming unimpeded even from the most remote corners of the universe, will enable researchers using the Hydrogen Epoch of Reionization Array to map the full 3D distribution of neutral gas in the universe.

RESULTS The team recently published findings which suggest that the global average 21-centimeter line signal was likely substantially weaker, when the universe was roughly one-tenth its current size, than predicted by an earlier analytical model. This affects the sensitivity requirements of upcoming surveys designed to detect that signal. They note, as well, that surveys designed to look for patterns in the clustering of matter should account for the 21-centimeter signal emanating from dense sub-structures.

The Fermilab researchers also found that their simulated model galaxies have many properties (such as light output, sizes, rates of star formation, spatial distribution, etc.) that agree well with the recent observations from the Hubble Space Telescope. Meeting another of its objectives, the team was able to reproduce the observed properties of intergalactic gas through simulations.

IMPACT With a better understanding of cosmic reionization, researchers will be able to shed light on other aspects of modern cosmology, from probing the nature of dark matter and dark energy through cosmic microwave background observations, to observing the physical state of intergalactic gas in the absorption spectra of high redshift quasars.

INCITE
150 Million Core-Hours
(ALCF: 80M; OLCF: 70M)
Physics



COSMOLOGICAL SIMULATIONS FOR LARGE-SCALE SKY SURVEYS

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Image Dark matter halo distribution from the Outer Rim simulation carried out on 32 racks of Mira with HACC. Shown is the full simulation volume with halos. Above a certain mass, halos are displayed as spheres colored with respect to mass. The light orange sphere is the heaviest. These halos host the galaxies that we observe with large telescopes.

Image credit: Joseph A. Insley and Silvio Rizzi, Argonne National Laboratory

Large-scale sky surveys are key drivers of advances in modern cosmology. This INCITE project relies on advanced computational tools to build accurate emulators to help resolve the mysteries of dark energy and dark matter. The simulations generate realistic synthetic observations and sky catalogs to help constrain a host of systematic uncertainties.

APPROACH This collaborative INCITE project focuses on two main areas in computational cosmology, both of which rely on the Hardware/Hybrid Accelerated Cosmology Code (HACC): the generation of cosmic emulators, precision prediction tools for different cosmological observables spanning a large range of parameters; and the construction of sophisticated synthetic sky maps from very large high-resolution cosmological simulations.

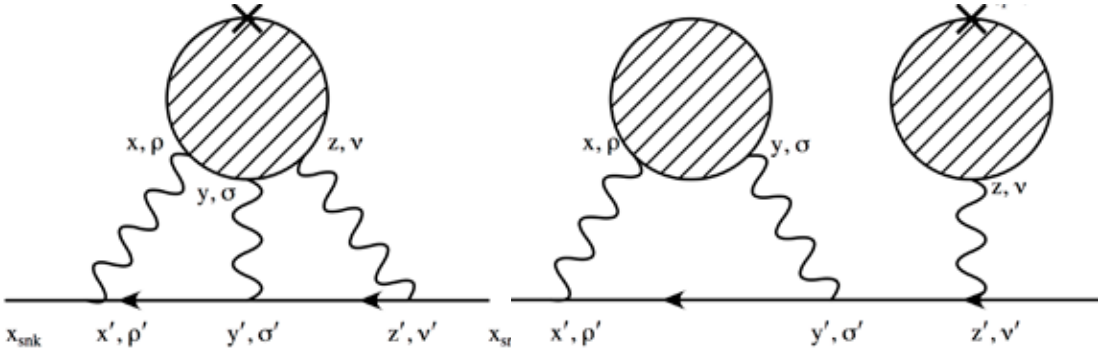
The team developed and continues to refine the Portal for Data Analysis services for Cosmological Simulations (PDACS) to enable the sharing of processed data from the project's Outer Rim simulation. Carried out on Mira, it evolved more than one trillion particles modeling the distribution of matter in the universe.

RESULTS The first set of simulations for cosmologies includes the effects of neutrinos and dynamical dark energy, an important extension of the current cosmological model to be confronted by next-generation sky surveys. With more than 45 models developed to date, these simulations will be part of the complete Mira-Titan Universe suite that will provide high-accuracy emulators for a variety of cosmological summary statistics. Analysis, so far, is focused on the matter power spectrum, redshift space distortions, the halo mass function, and the halo concentration-mass relation.

In addition, simulations aid ongoing and future surveys by creating synthetic sky maps, which underlie data challenges for the Dark Energy Science Collaboration of the Large Synoptic Survey Telescope project. Maps were also created to investigate the Sunyaev-Zel'dovich effect—a distortion of the thermal cosmic microwave background (CMB) photon spectrum—to aid in the cross-correlation of CMB measurements from the South Pole Telescope and the Dark Energy Survey.

IMPACT This research provides the computational tools and expertise to run frontier simulations and analyses on the CMB and large-scale structure observables, such as the mass distribution in the universe.

ALCC
175 Million Core-Hours
Physics



HADRONIC LIGHT-BY-LIGHT SCATTERING CONTRIBUTION TO THE MUON ANOMALOUS MAGNETIC MOMENT

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University of Connecticut

Image Hadronic light-by-light scattering contributions to the muon g-2, quark-connected loop (left) and quark-disconnected loops (right). The loops are made of quarks and represent hadronic states generated through the exchange of virtual gluons (not shown), including those connecting the two quark loops on the right.

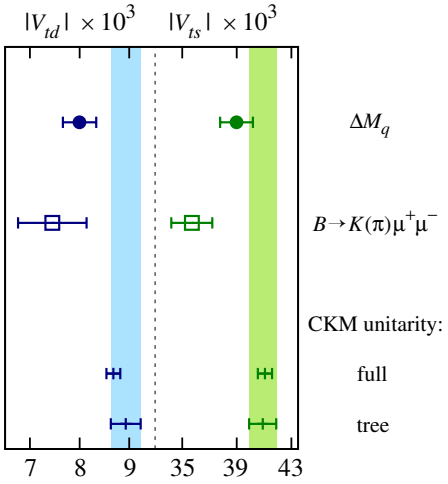
Image credit: Thomas Blum, University of Connecticut

The muon anomalous magnetic moment (muon g-2) presently provides the most compelling hint for new physics beyond the Standard Model, but experiment and theory currently disagree by three standard deviations. Calculations performed in support of the muon g-2 experiment at Fermilab are aimed at reducing theory errors which arise from quantum chromodynamics (QCD). This INCITE project enables an important step towards a complete, controlled calculation of the hadronic light-by-light contribution in lattice QCD.

APPROACH The muon g-2 experiment is regarded as one of the most important DOE Intensity Frontier experiments. Using Fermilab's proton accelerators and ALCF's computational resources, this experiment will explore the interactions of muons in strong magnetic fields, while reducing experimental uncertainty. The largest theory errors arise from hadronic contributions (i.e., quarks and gluons), specifically, the hadronic vacuum polarization in QCD, and hadronic light-by-light (HLbL) scattering. Researchers hope to reduce the experimental errors by a factor of four to determine whether known discrepancies are a sign of new physics, or just statistical fluctuation. Current work involves calculating the HLbL scattering contribution, which involves quarks exchanging photons with muons. Models for this contribution have uncertainties of about 25-40 percent.

RESULTS Performing first-principles calculations using lattice QCD methods, the team originally proposed to calculate the dominant proponent of the HLbL scattering contribution with statistical errors of around 20 percent. The team has since passed its original project goal, achieving about 11 percent. To achieve these goals at physical masses, new numerical techniques were developed that dramatically reduced the cost of the calculations. These include all mode averaging, the zMöbius formulation of the lattice Dirac operator, and a new method for computing the light-by-light amplitude. To compliment these, they employed an optimized Bagel/BFM code, which sustains 15 percent of peak speed on Mira for production runs on the ensemble of QCD gauge configurations being used.

IMPACT These calculations will have a large impact on theoretical results, paving the way for further refinements and, eventually aiding in the search for new fundamental physics beyond the Standard Model. If new physics are detected at the Large Hadron Collider, the muon anomalous magnetic moment, if confirmed, will be crucial to understanding the source.



LATTICE QCD

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Fermilab

Image Values of CKM matrix elements obtained from processes mediated by quantum loops, such as B-meson mixing (ΔMq) and B neutral current decays (such as B→K(π) μμ), lie systematically below those obtained from processes not mediated by loops (colored bands). This is a possible indication of physics beyond the Standard Model.

Image credit: Fermilab Lattice and MILC Collaborations

Despite the acceptance and application of the Standard Model of physics, physicists believe that a more general theory will be needed to explain physics at the shortest length scales, or highest energies. This project aims to dramatically advance research in lattice quantum chromodynamics (QCD) and other strongly coupled field theories to search for new physics beyond the Standard Model.

APPROACH For this project, researchers from the USQCD Collaboration are advancing exploration in lattice QCD, the theory of the strong interactions between quarks and gluons, which constitute hadrons, such as protons, neutrons, and pions. Supercomputers like Mira have made it possible, for the first time, to perform calculations at the physical value of the pion mass on very fine lattices.

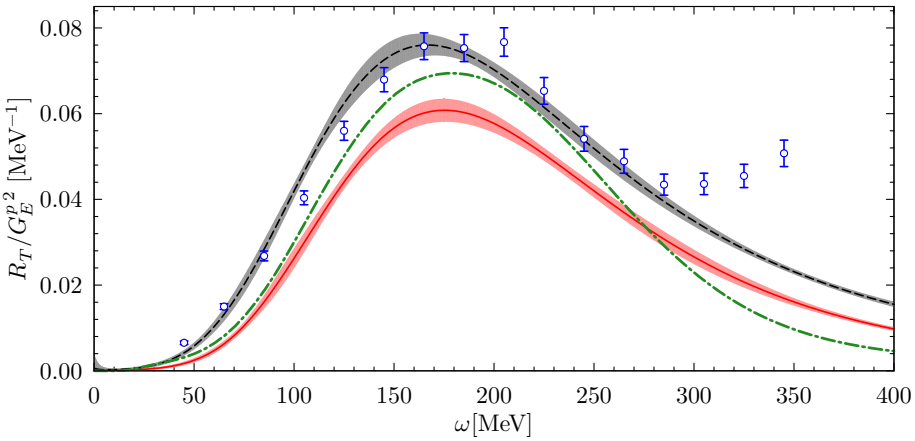
RESULTS Recently, researchers from the Fermilab Lattice and MILC Collaborations, a subgroup of the larger project, calculated a complete description of neutral B-meson mixing on a background of lattice QCD configurations with three flavors of quarks (up, down, and strange). This was the first such calculation to incorporate a complete parameterization of all possible effects contributing to this mixing, both within and beyond the Standard Model. In the Standard Model, B mixing is mediated by quantum loops, which are suppressed. This is expected to make possible effects of physics beyond the Standard Model easier to see in such processes. The researchers found that when they used new results to extract fundamental parameters of the Standard Model (CKM quark mixing matrix elements), they obtained values lower than those found in processes not mediated by loops, pointing to the possibility of new physics. More precise calculations will be needed to determine whether this is the case.

IMPACT Researchers believe that the relationship between particles operating within this specific mixing may be sensitive to interactions with new undiscovered particles and may suggest the occurrence of effects of physics beyond the Standard Model. Furthermore, the discovery of a true discrepancy between Standard Model predictions and experiment would lay the foundation for a new era in particle physics.

INCITE

184 Million Core-Hours (ALCF: 80M; OLCF: 104M)

Physics



NUCLEAR STRUCTURE AND NUCLEAR REACTIONS

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Iowa State University

Image Electromagnetic transverse response of carbon-12 at (top to bottom) momentum transfers of 300, 380, and 570 MeV/c.

Image credit: Reproduced from *Physical Review C*, DOI: 10.1103/PhysRevC.91.062501 (2016)

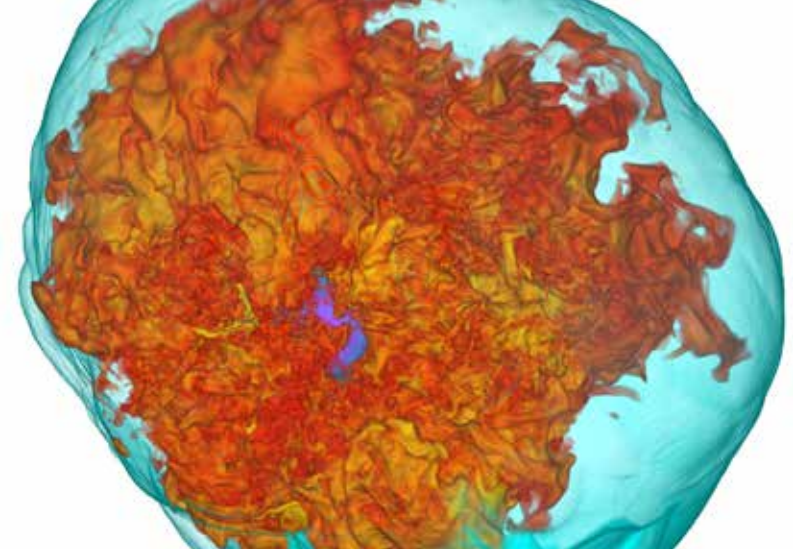
The development of a robust and precise nuclear theory, based on the Standard Model of elementary particles interacting through strong and electroweak forces, represents a "holy grail" for physics. Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs. But developing such a theory requires investigations of exotic isotopes that are difficult or impossible to study experimentally. For this INCITE project, a multi-institution research team is using DOE supercomputers to provide more accurate predictions.

APPROACH As part of the project, researchers from Argonne National Laboratory are using Green's function Monte Carlo (GFMC) to calculate electroweak interactions of light nuclei, specifically helium-4 and carbon-12, the most common of the carbon isotopes. The electroweak response—interactions mediated by either electromagnetic or weak nuclear forces—is important in describing how a neutrino scatters off of carbon-12. As a first step towards the neutrino scattering calculation, the team has computed the electromagnetic response of carbon-12. Work will also begin on neutrino scattering to the first isospin -1 state of carbon-12; these calculations will be important for both neutrino detector calibrations and supernova simulations.

RESULTS Last year, the team used GFMC propagation methods to compute the Euclidean response functions of electromagnetic and neutral weak currents in helium-4 and carbon-12 at low and moderate values of momentum transfer. Excellent results were obtained when the team inverted the carbon-12 electromagnetic response. Continued work on inverting the neutral-weak responses of carbon-12 will allow for the resolution of the axial mass puzzle, a discrepancy between experiment and theory in determining the strength of the neutrino-nucleus interactions.

IMPACT Accurate predictions that better illustrate nuclear structure and nuclear reactions are important to many applications in nuclear energy, including the future development of advanced fission reactors and fusion energy. They are also relevant to DOE's current and planned user experimental facilities, such as Jefferson Lab and the Facility for Rare Isotope Beams, where new phenomena and precision tests of the Standard Model are anticipated.

INCITE
50 Million Core-Hours
Physics



PETASCALE SIMULATION OF **MAGNETOROTATIONAL CORE-COLLAPSE SUPERNOVAE**

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Michigan State University

Image This image is from a 3D magnetohydrodynamics simulation of a rapidly rotating, highly magnetized star.

Image credit: Sean Couch, Michigan State University

The process by which core-collapse supernovae (CCSN) are produced drives the development of the heavier elements, which are distributed throughout the universe after a massive star explodes under its own weight. Project researchers will conduct a comprehensive study of the mechanisms that cause core-collapse supernovae utilizing 3D magnetohydrodynamics simulations of the collapse of rotating, magnetic stellar cores.

APPROACH The research team is achieving high-level views of magnetohydrodynamic turbulence using the multiphysics FLASH code on Mira, as well as a sophisticated two-moment neutrino transport scheme with an analytic closure for higher-order moments. Known as M1, the code was refactored, resulting in a performance increase of nearly 50 percent and better coupling of the M1 transport to the hydrodynamics.

The team ran two 3D simulations with the M1 high-fidelity neutrino transport using a state-of-the-art 20-solar mass (20 times the mass of our own sun) 1D progenitor model generated by the MESA code. One simulation used non-spherical velocity perturbations in the silicon- and oxygen-burning shells, and the other did not. Due to the M1 code optimization, they have achieved higher resolutions than originally planned.

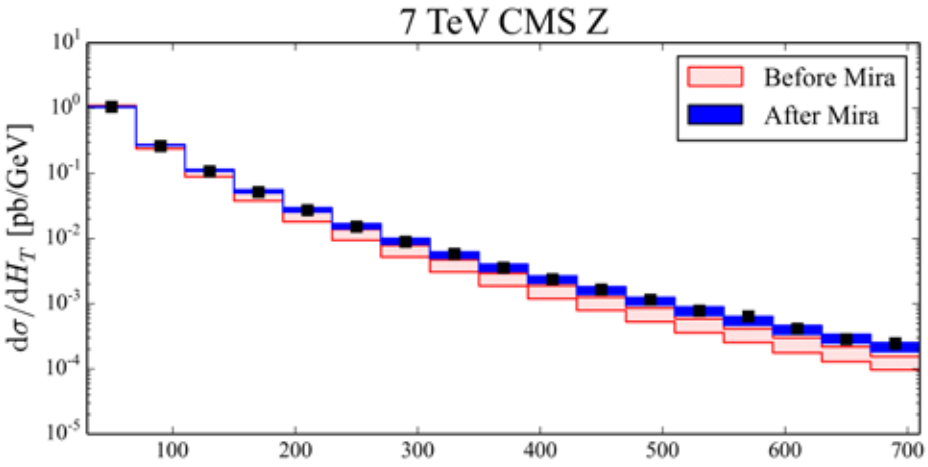
RESULTS Based on a large set of high-resolution, 3D CCSN simulations carried out exclusively on Mira, the team demonstrated that the creation of successful explosions relies on strong turbulent pressure behind the shock and the presence of strong non-spherical motion in the pre-collapse progenitor star. This work emphasized the importance of turbulence in the supernova mechanism.

New simulations will allow researchers to probe the behavior and importance of turbulence in aiding supernova shock revival in the most realistic way yet, particularly in conjunction with simulations that include non-spherical progenitor perturbations.

IMPACT Project research will allow for the prediction of the spins, kicks, magnetic field strengths and alignments of newly formed neutron stars, pulsars, and magnetars, as well as the dependence of these parameters on progenitor conditions. These simulations will be the most physically detailed and accurate CCSN simulations to include magnetorotational effects ever accomplished, with the potential for uncovering a robust and realistic CCSN explosion mechanism.

DIRECTOR'S DISCRETIONARY

9 Million Core-Hours
Physics



PREDICTING THE TERASCALE ON-DEMAND WITH HIGH-PERFORMANCE COMPUTING

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Argonne National Laboratory

Image Demonstration of the enhanced agreement between LHC experimental data (black data points) and theory after simulating the vector boson jet process on Mira (blue bands), compared to agreement before Mira simulations (black data points and red bands).

Image credit: Radja Boughezal, Argonne National Laboratory

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

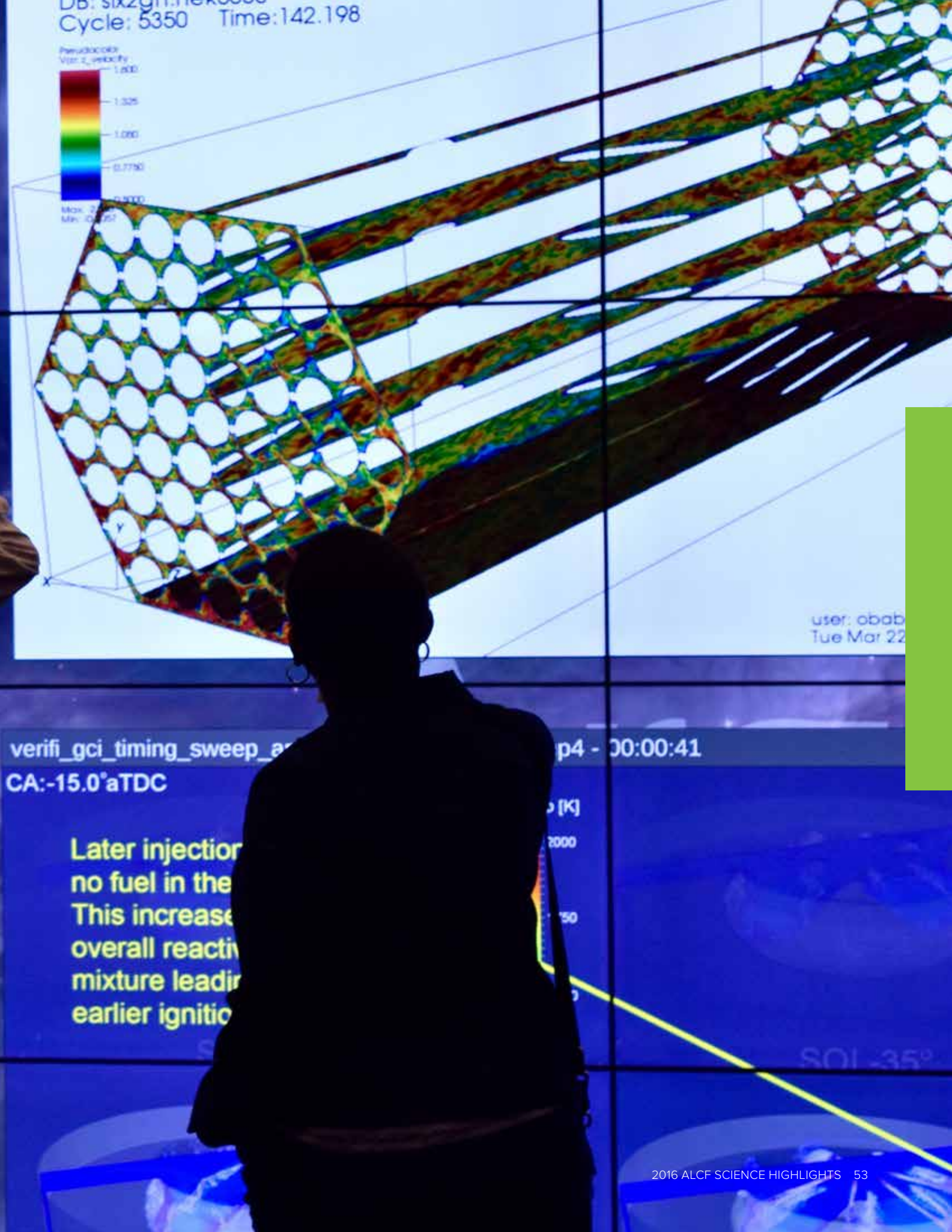
APPROACH In this large-scale computational study, researchers from Argonne National Laboratory developed a novel framework adapted for supercomputers to perform precision calculations that are critical to advancing knowledge of phenomena such as dark matter. They used two-thirds of Mira's more than 49,000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

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

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

ALCF RESOURCES

The ALCF's unique combination of expertise and supercomputing resources helps researchers solve some of the world's largest and most complex problems.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no fuel in the
This increase
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earlier ignitio

79
STAFF MEMBERS

15
POSTDOCTORAL RESEARCHERS

22
SUMMER STUDENTS

ALCF EXPERTISE

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

Catalyst

The Catalyst team is comprised of computational scientists who work directly with project teams to maximize and accelerate their research efforts.

Data Analytics and Visualization

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

Data Science

The Data Science team is focused on developing and improving computational methods to enable users to productively solve data-centric science challenges on current and future ALCF systems.

Operations

Responsible for the day-to-day operations of ALCF systems, the Operations team brings extensive experience in all aspects of HPC hardware and software, including advanced integration, system and network administration, infrastructure, and storage.

Performance Engineering

The Performance Engineering team helps 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.

User Experience

The User Experience team supports the ALCF user community by providing technical assistance, outreach and training, and public awareness of research conducted at the facility.

ALCF 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. 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
- 49,152 nodes
- 16 1600 MHz PowerPC A2 cores per node
- 786,432 cores
- 768 TB RAM
- 5D torus interconnect
- 384 I/O nodes
- Peak performance of 10 petaflops

CETUS

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

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

VESTA

As the ALCF's test and development platform, Vesta serves 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 TB RAM
- 5D torus interconnect
- 32 I/O nodes
- Peak performance of 419 teraflops

ALCF users have access to several computing resources, including one of the most powerful supercomputers in the world.

COOLEY

Cooley is the ALCF's analysis and visualization cluster. Equipped with graphics processing units (GPUs), Cooley converts computational data from Mira into high-resolution visual representations. The resulting images and videos help users to better analyze and understand the data generated by Mira. Cooley 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. Cooley shares file systems with Mira, enabling direct access to Mira-generated results.

Each Cooley node has:

- Two 2.4 GHz Intel Haswell E5-2620 v3 6-core processors
- NVIDIA Tesla K80 GPU with 24 GB GPU RAM
- 384 GB RAM

The full Cooley system has:

- 126 nodes
- 1,512 cores
- FDR Infiniband interconnect
- 47 TB RAM
- 3 TB GPU RAM
- Peak performance of 293 teraflops

DATA STORAGE

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

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

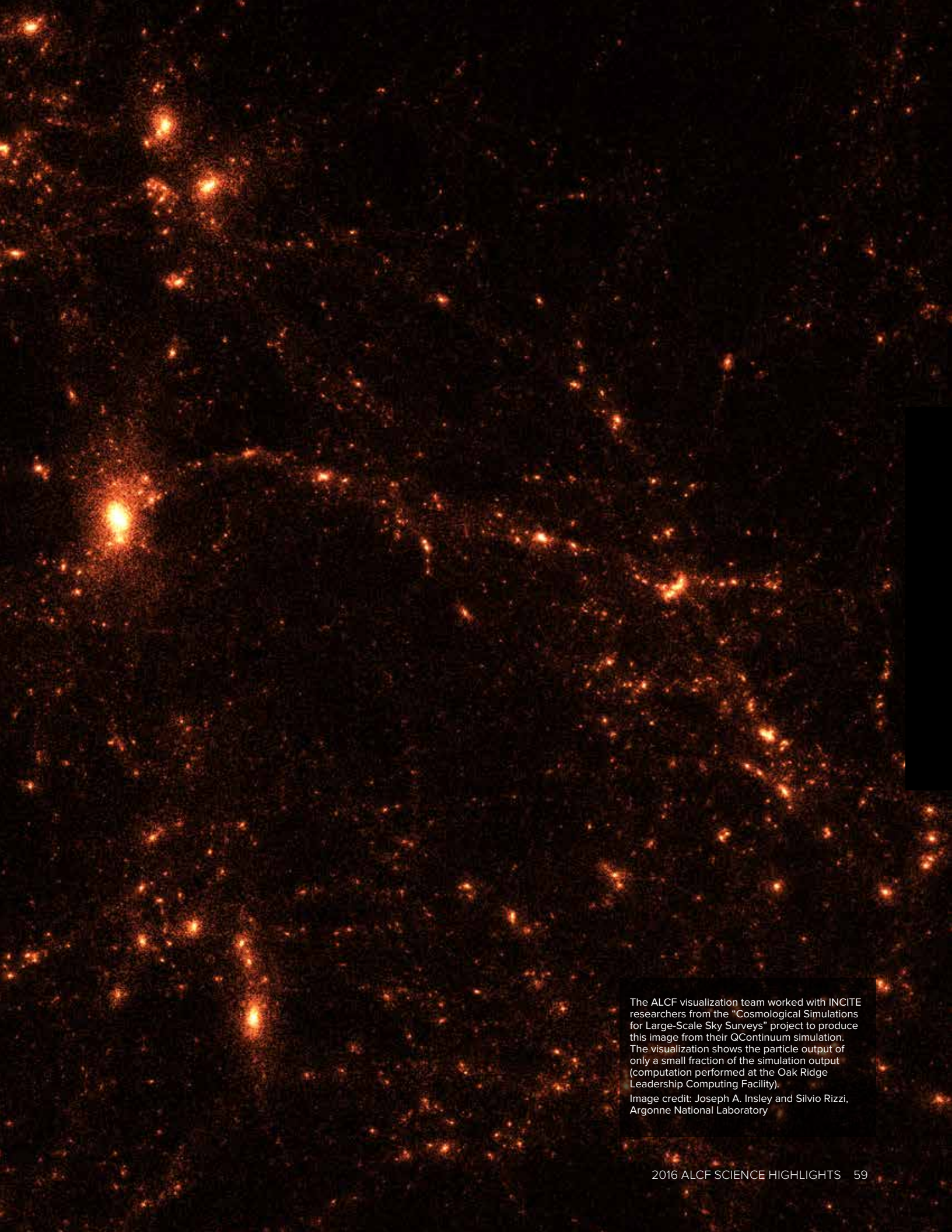
TAPE STORAGE The ALCF has two 10,000-slot libraries using LTO 6 tape technology. The LTO tape drives have built-in hardware compression with compression ratios typically between 1.25:1 and 2:1, depending on the data, giving an effective capacity of 26-40 PB.

NETWORKING

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

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

2016 PROJECTS



The ALCF visualization team worked with INCITE researchers from the "Cosmological Simulations for Large-Scale Sky Surveys" project to produce this image from their QContinuum simulation. The visualization shows the particle output of only a small fraction of the simulation output (computation performed at the Oak Ridge Leadership Computing Facility).

Image credit: Joseph A. Insley and Silvio Rizzi, Argonne National Laboratory

ALCF PROJECTS

2016 INCITE PROJECTS

Biological Sciences

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

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

Chemistry

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

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

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

Computer Science

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

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

Earth Science

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

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

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

Engineering

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

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

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

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

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

Materials Science

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

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

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

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

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

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

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

SiO_2 Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme
James Kermode, University of Warwick
126 Million Core-Hours

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

Unveiling the Behavior of UO_2 Under Extreme Physical Conditions
Peter Littlewood, Argonne National Laboratory
75 Million Core-Hours

Physics

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

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

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

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

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

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

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

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

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

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Chemistry

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

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

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

Computer Science

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

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

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

Earth Science

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

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

Engineering

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

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

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

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

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

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

Materials Science

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

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

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

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

Physics

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

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

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

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

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

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

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Biological Sciences

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

Chemistry

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

Computer Science

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

Earth Science

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

Engineering

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

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

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

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

Materials Science

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

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

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

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

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

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

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

Physics

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

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

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

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

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

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

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

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

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

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

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

2016 Director's Discretionary Projects

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

Biological Sciences

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

Chemisty

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

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

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

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

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

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

Computer Science

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

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

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

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

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

Earth Science

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

Engineering

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

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

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

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

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

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

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

Materials Science

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

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

Physics

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

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

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

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

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

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

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

About Argonne Leadership Computing Facility

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

About Argonne National Laboratory

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