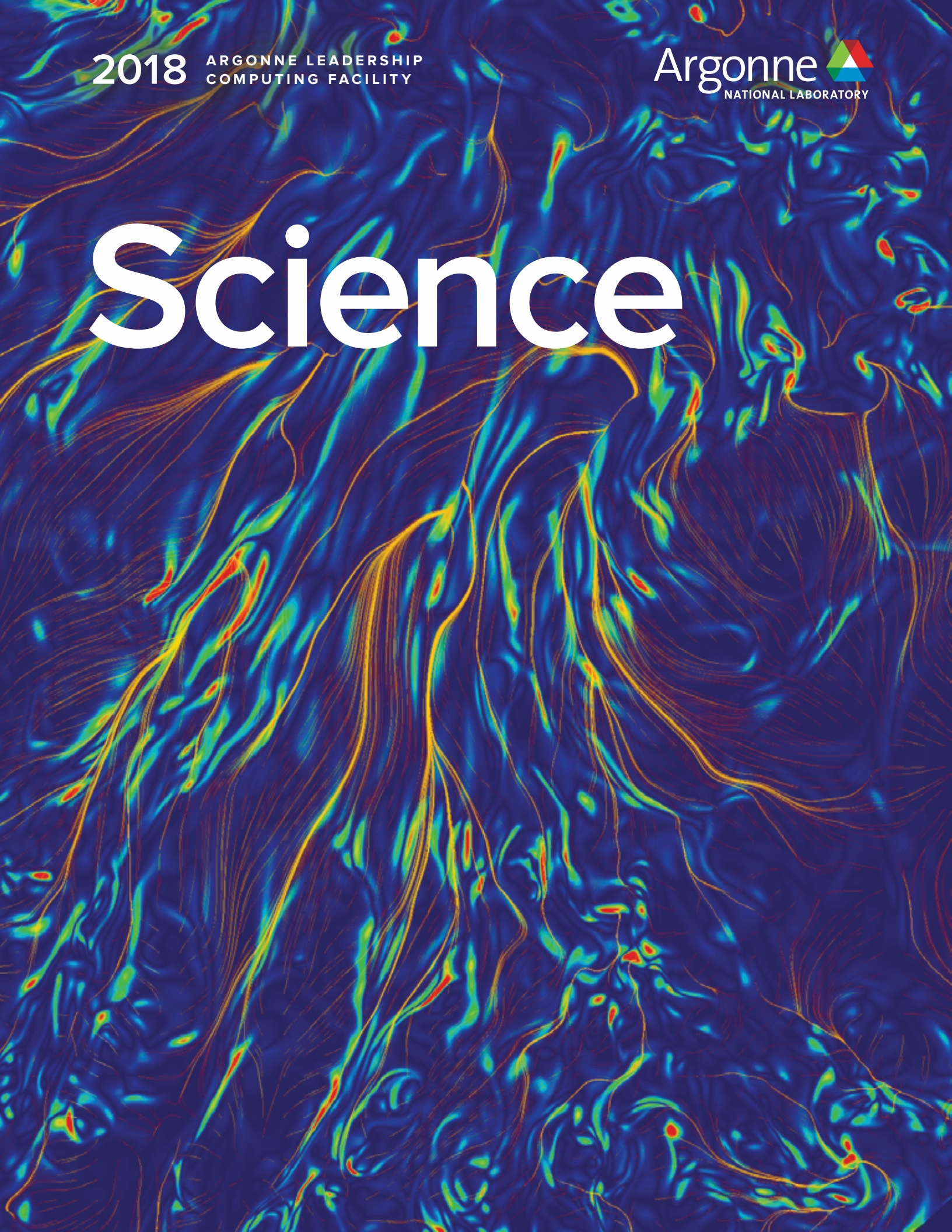
2018 ARGONNE LEADERSHIP COMPUTING FACILITY

Argonne NATIONAL LABORATORY

Science



A zoomed-in portion of a visualization showing the boundary layer structure right at the heated bottom plate of a cylindrical cell for turbulent Rayleigh-Bénard convection in liquid sodium.
Image: Joerg Schumacher, Technische Universitaet Ilmenau

2018 SCIENCE CONTENTS

SCIENCE DIRECTOR'S MESSAGE

Katherine Riley
Director of Science

This year sees the ALCF looking forward. As we prepare to enter the exascale era, the future of leadership computing lies in simulation, data, and learning. To best support this paradigm, we are striving to direct our efforts to develop the facility so that its growth synergizes with our users' research.

In 2018, we expanded the Aurora Early Science Program (ESP), adding data analysis and machine learning projects to the simulation-based projects already underway.

Collectively, these projects cover various combinations of techniques and approaches across a wide range of disciplines and goals. Common to all of them, though, is a substantial data challenge: at this point in computational science, data problems are no longer unique to projects that explicitly identify as such.

The ALCF Data Science Program (ADSP) is yet another way we support projects that rely on advanced computational methods to enable data-driven discoveries. In addition, this year marked the first time that the INCITE program has explicitly sought data- and learning-based projects as part of its annual call for proposals.

Partnering with the research teams supported by these programs allows us to take a collaborative approach to exploring not simply how to elevate the roles of data in computational science, but how to strike the appropriate balance between them and construct an architecture readily adaptable to each project's needs.

The exemplary work being done at the ALCF today is critical to advancing our transition into a facility that fully supports a new class of capabilities. Projects such as the ADSP-supported efforts of University of Cambridge researchers to develop solar power-generating windows by mining published papers to identify potential materials are what allow us to tackle the problems and solutions that will define the next phase of supercomputing.

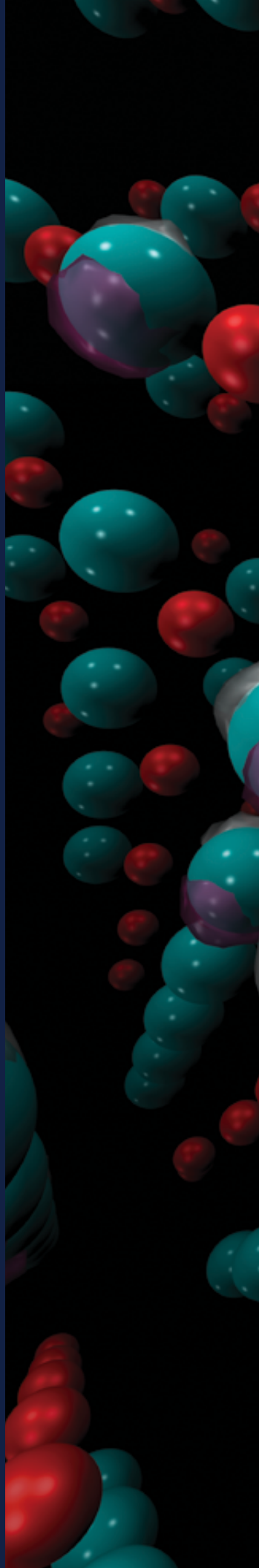
Aurora itself will introduce new and novel ways to approach computational science and engineering research. Along the way, exciting ancillary technologies and services like Singularity and Balsam are being introduced to make the ALCF ever more compatible with users' requirements and preferences.

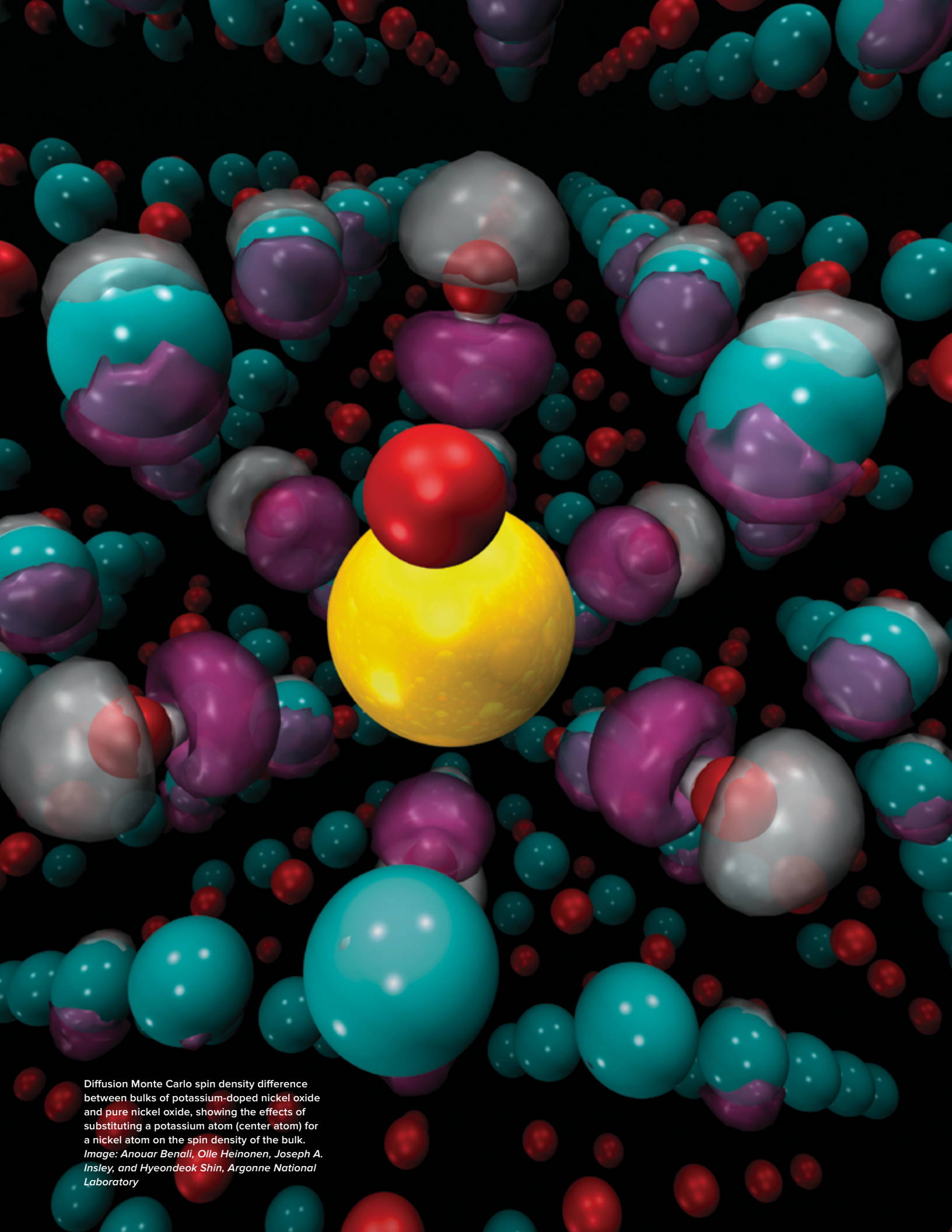
To help the ALCF community take advantage of these emerging tools and frameworks, we remain committed to providing training opportunities that educate our users about the resources available to them. As part of this year's many offerings, we hosted two workshops on combined simulation, data, and learning topics to help our users improve their code performance and productivity on our systems.

These efforts are helping us to drive a new paradigm for scientific computing that will accelerate discoveries and innovations in the exascale era. We are excited for what the future holds.

ARGONNE LEADERSHIP COMPUTING FACILITY

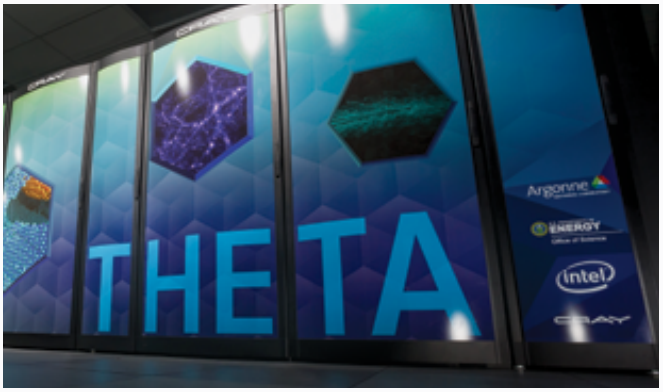
The ALCF enables breakthroughs in science and engineering by providing supercomputing resources and expertise to the research community.





Diffusion Monte Carlo spin density difference between bulks of potassium-doped nickel oxide and pure nickel oxide, showing the effects of substituting a potassium atom (center atom) for a nickel atom on the spin density of the bulk. *Image: Anouar Benali, Olle Heinonen, Joseph A. Insley, and Hyeondeok Shin, Argonne National Laboratory*

About ALCF



With a peak performance of more than 11 petaflops, the ALCF's Theta system is among the fastest supercomputers in the world for open scientific research.

The Argonne Leadership Computing Facility (ALCF) is a national scientific user facility that provides supercomputing capabilities to the scientific and engineering community to accelerate the pace of discovery and innovation in a broad range of disciplines.

As a key player in the nation's efforts to deliver future exascale computing capabilities, the ALCF is driving the convergence of simulation, data science, and machine learning to advance scientific computing.

Available to researchers from universities, industry, and government agencies, ALCF computing resources 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 computing projects aimed at solving some of the world's largest and most complex problems in science and engineering.

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.

ALCF Team

The ALCF's talented and diverse staff make the facility one of the world's premier centers for scientific computing.

Operations
HPC systems administrators manage and support all ALCF computing systems, network infrastructure, storage, and systems environments, ensuring that users have stable, secure, and highly available resources to pursue their scientific goals. HPC software developers create and maintain a variety of tools that are critical to the seamless operation of the ALCF's supercomputing environment. Operations staff members also provide technical support to research teams, assimilate and verify facility data for business intelligence efforts, and generate documentation to communicate policies and procedures to the user community.

Science and Technology
Experts in computational science, performance engineering, data science, machine learning, and scientific visualization work directly with users to maximize and accelerate their research efforts on the facility's computing resources. With multidisciplinary domain expertise, a deep knowledge of the ALCF computing environment, and experience with programming methods and community codes, the ALCF's in-house researchers ensure that users are able to meet their science goals.

Outreach
Staff outreach efforts include facilitating partnerships with industry, coordinating user training events, and participating in educational activities. Staff members also communicate the impact of facility research and innovations to external audiences through reports, promotional materials, science highlights, and tours.

ALCF Computing Systems

Mira

Mira is the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer.

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

Theta

Theta is the ALCF's 11.69-petaflops Intel-Cray supercomputer.

- Intel-Cray XC40 architecture
- 11.69 petaflops
- 64-core, 1.3-GHz Intel Xeon Phi 7230 processor per node
- 4,392 nodes
- 281,088 cores
- 843 TB of memory
- 70 TB of high-bandwidth memory
- Aries interconnect with Dragonfly configuration
- 24 racks

Cetus

Cetus is an IBM Blue Gene/Q system used to offload both debugging issues and alternative production workloads from Mira.

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

Iota

Iota serves as the ALCF's Intel-Cray test and development platform.

- Intel-Cray XC40 architecture
- 117 teraflops
- 64-core, 1.3-GHz Intel Xeon Phi 7230 processor per node
- 44 nodes
- 2,816 cores
- 12.3 TB of memory
- 1 TB of high-bandwidth memory
- Aries interconnect with Dragonfly configuration
- 1 rack

Vesta

Vesta serves at the ALCF's IBM Blue Gene/Q test and development platform.

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

Cooley

Cooley is the ALCF's data analysis and visualization cluster.

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

Supporting Resources

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 Mira system consists 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. Mira uses the General Parallel File System (GPFS) to access the storage. The Theta system consists of 30 I/O nodes that connect to a storage array that controls 2,300 disk drives with a total useable capacity of 9 PB and a maximum aggregate transfer speed of 240 GB/s. Theta uses Lustre to access this storage.

TAPE STORAGE

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

Networking

The Mira and Theta systems each 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 ESnet and Internet2.

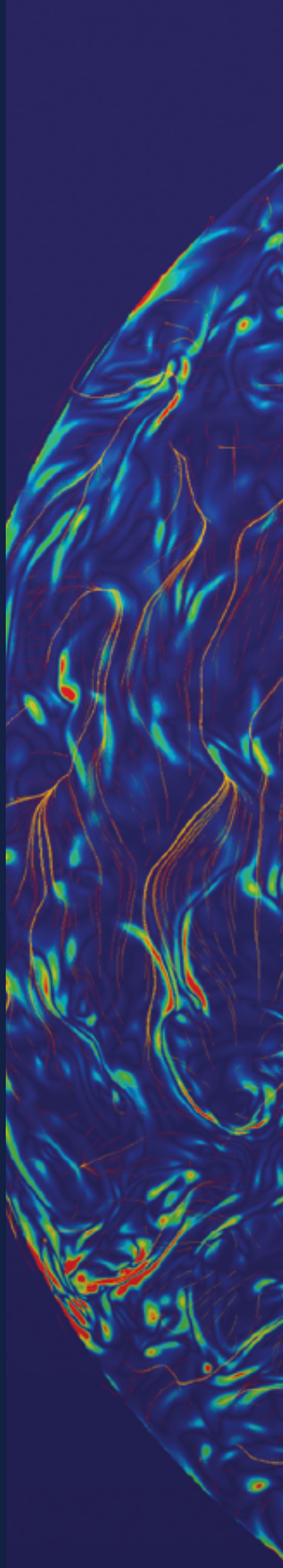
Testbeds

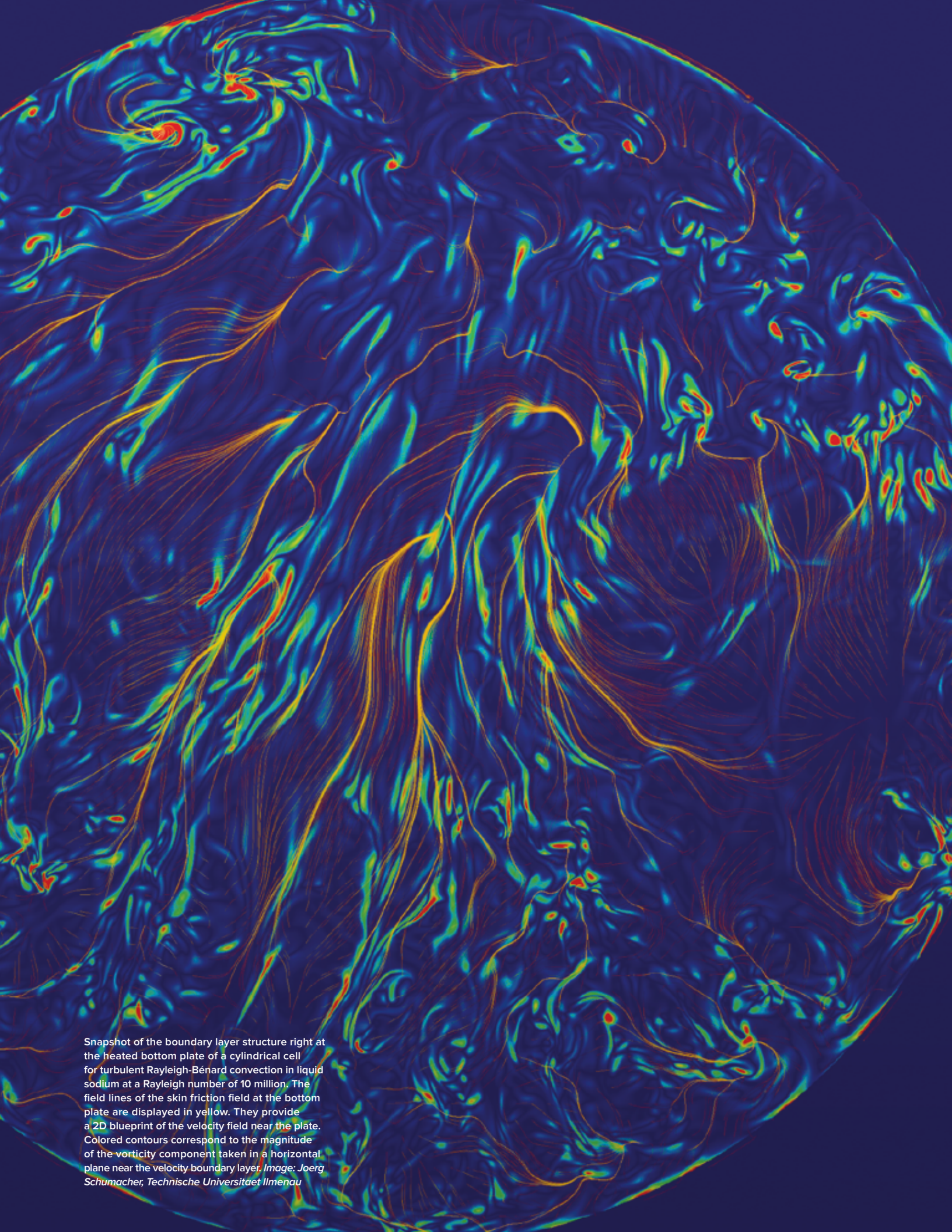
Through Argonne's Joint Laboratory for System Evaluation, the ALCF provides access to next-generation hardware and software to explore low-level experimental computer and computational science, including operating systems, messaging, compilers, benchmarking, power measurements, I/O, and new file systems. These include:

Intel Xeon Phi Knights Landing Cluster	**HPE Comanche Prototype ARM64 Cluster**
IBM Power System S822LC	**Kubernetes Cluster with Rancher**
Atos Quantum Learning Machine	**NVIDIA DGX–1**
Intel Xeon Platinum Skylake Cluster	**IBM Elastic Storage Server GL6**

REDEFINING HPC

As a key player in the nation's efforts to deliver future exascale systems, the ALCF is driving the convergence of simulation, data science, and machine learning to advance scientific computing.





Snapshot of the boundary layer structure right at the heated bottom plate of a cylindrical cell for turbulent Rayleigh-Bénard convection in liquid sodium at a Rayleigh number of 10 million. The field lines of the skin friction field at the bottom plate are displayed in yellow. They provide a 2D blueprint of the velocity field near the plate. Colored contours correspond to the magnitude of the vorticity component taken in a horizontal plane near the velocity boundary layer. *Image: Joerg Schumacher, Technische Universitaet Ilmenau*

The High-Tech Evolution of Scientific Computing

The ALCF continues to expand beyond traditional simulation-based research, creating an environment that also supports emerging data science and machine learning approaches.

Realizing the promise of exascale computing, the ALCF is developing the framework by which to harness this immense computing power to an advanced combination of simulation, data science, and machine learning. This effort will undoubtedly reframe the way science is conducted, and do so on a global scale.

Since the ALCF was established in 2006, the methods used to collect, analyze, and employ data have changed dramatically. Where data was once the product of and limited by physical observation and experiment, advances in feeds from scientific instrumentation such as beamlines, colliders, and space telescopes—just to name a few—have increased data output substantially, giving way to new terminologies, like "big data."

While the scientific method remains intact and the human instinct to ask big questions still drives research, the way we respond to this new windfall of information requires a fundamental shift in how we use emerging computing technologies for analysis and discovery.

This convergence of simulation, data, and learning is driving an ever more complex but logical feedback loop.

Increased computational capability supports larger scientific simulations that generate massive datasets used to feed a machine learning process, the output of which informs further and more precise simulation. This, too, is further augmented by data from observations and experiments to refine the process using data-driven approaches.

While simulation has long been the cornerstone of scientific computing, the ALCF has been working to integrate data analysis and machine learning-based projects into the fold for the past few years.

To advance that objective, the facility launched its ALCF Data Science Program (ADSP) in 2016 to explore and improve computational methods that could better enable data-driven discoveries across scientific disciplines. The ALCF also recently expanded its Aurora Early Science Program with the addition of 10 new projects that will help prepare the facility's future exascale supercomputer for data and learning approaches.

And late last year, Argonne announced the creation of the Computational Science division and the Data Science and Learning division to explore challenging scientific problems through advanced modeling and simulation, and data analysis and other artificial intelligence methods, respectively.

Already, this combination of programs and entities is being tested and proved through studies that cross the scientific spectrum, from designing new materials for solar energy applications to deciphering the neural connectivity of the brain.

Built for Simulation, Data, and Learning

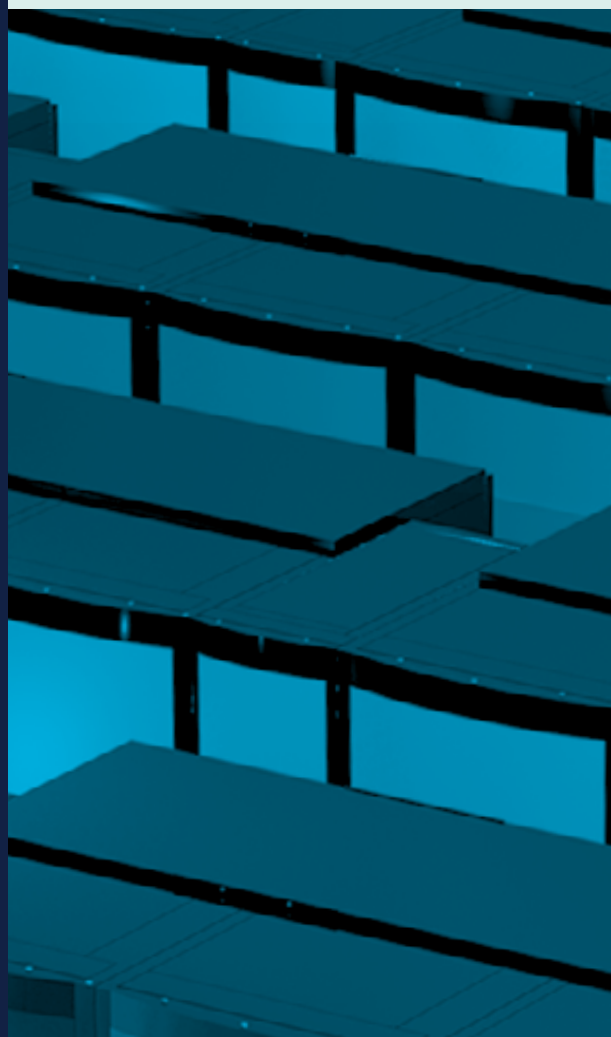
The merging of simulation, data, and learning is only possible because of the exponential and deliberate development of high-performance computing and data delivery systems.

Supercomputer architectures are now being structured to make them more amenable to dealing with large amounts of data and to facilitate learning, in addition to traditional simulations. And ALCF researchers are fitting these machines with massive conduits that allow them to stream large amounts of data from the outside world, like the Large Hadron Collider at CERN and Argonne's Advanced Photon Source (APS), and to enable data-driven models.

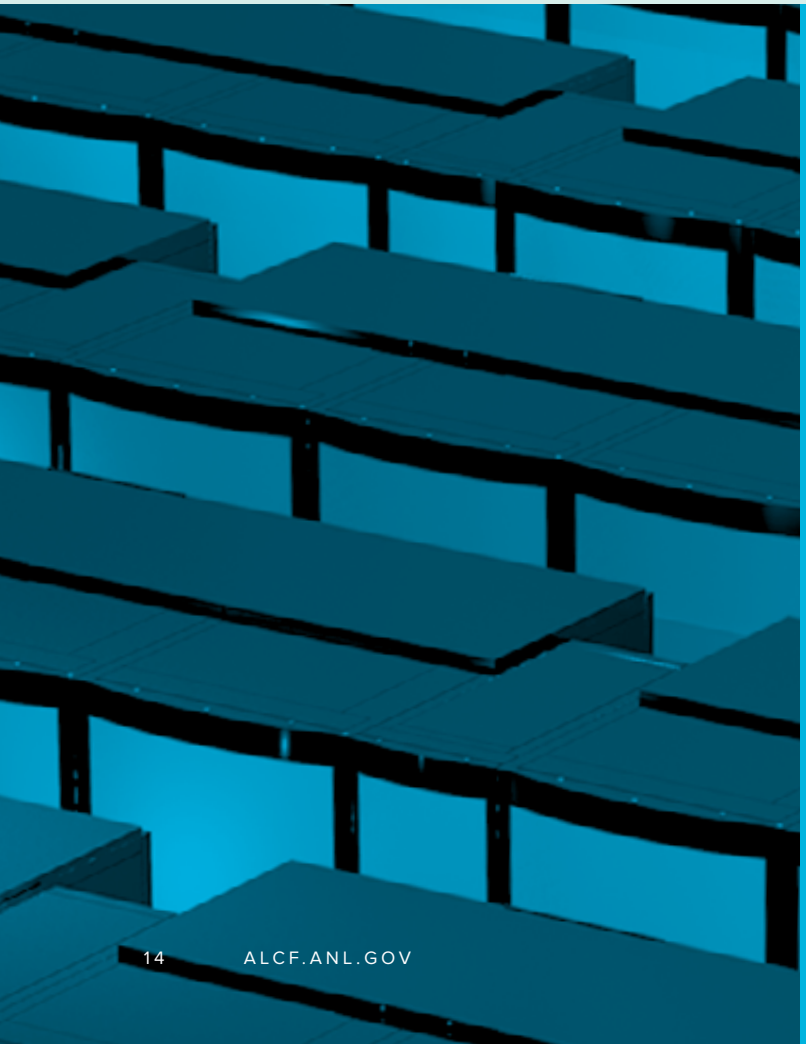
Many current architectures still require the transfer of data from computer to computer, from one machine, the sole function of which is simulation, to another that excels in data analysis and/or machine learning.

Within the last few years, Argonne and the ALCF have made a significant investment in high-performance computing that gets them closer to a fully integrated machine. The process accelerated in 2017, with the introduction of the Intel-Cray system, Theta, which is capable of combining traditional simulation runs, data analysis, and machine learning techniques.

The ALCF will help drive simulation, data, and learning to a new level in 2021, when they unveil Argonne's first exascale machine, Aurora. While it can perform a billion



Simulation Data Learning



Simulation

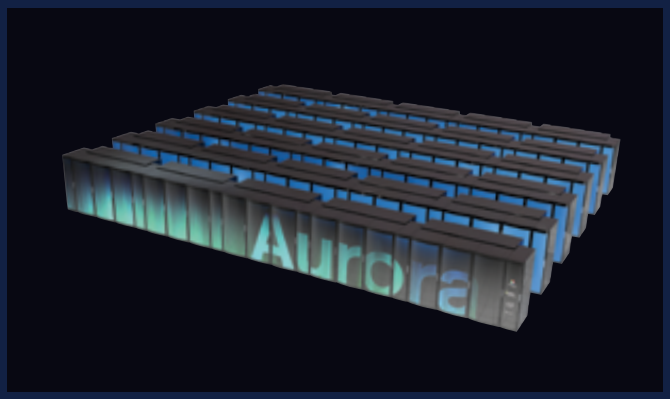
Simulation allows researchers to create virtual representations of complex physical systems or processes that are too small or large, costly, or dangerous to study in a laboratory.

Data

The use of advanced data science techniques and tools to gain insights into massive datasets produced by experimental, simulation, or observational methods.

Learning

A form of artificial intelligence, machine learning refers to a set of algorithms that uses training data to identify relationships between inputs and outputs, and then generates a model that can be used to make predictions on new data.



Argonne's first exascale system, Aurora, will help ensure continued U.S. leadership in high-end computing for scientific research.

billion calculations per second, its main advantage may be its ability to conduct and converge simulation, data analysis, and machine learning. The end result will allow researchers to approach new types of problems on a much larger scale and reduce time to solution.

Advancing Science with Data-Centric Tools and Services

While data has always been an integral part of scientific computing, the ever-growing amount of data being produced by large-scale simulations, telescopes, light sources, and other experimental facilities calls for new technologies and techniques for analysis and discovery.

To align with these emerging research needs, the ALCF continues to explore and deploy new data-centric tools that take advantage of the advanced computing capabilities provided by its leadership computing resources, allowing users to extend their work to large-scale science campaigns involving petabytes of data.

The goal is to drive advances in scientific machine learning and big data analytics by providing facility users with high-performing, scalable machine learning software, analytics frameworks, data management services, workflow packages, and runtime optimizations. This includes custom-built software tools designed for specific tasks, as well as open-source software tools adapted to meet various research needs.

However, deploying and operating a big data software stack on a system of Theta's scale is not a trivial task. The ALCF has assembled a suite of data science and machine learning frameworks and tools specifically optimized to exploit the Intel-Cray system's capabilities. ALCF staff members have built these tools to utilize Intel-optimized libraries and Intel's Python distribution, which maximize the use of Theta's unique massively parallel, many-core system architecture, compute power, and high-speed interconnect.

This is part of a continuing effort to expand the ALCF's scope beyond that of a traditional high-performance computing facility. In addition to providing resources to enable data-driven discoveries, the ALCF's evolving suite of services and tools aims to help to eliminate barriers to productively using the facility's systems, integrate with user workflows to produce seamless, usable environments, and enhance collaboration among research teams.

Preparing Aurora for Science on Day One

Through the ALCF's Aurora Early Science Program, 15 project teams are preparing to be among the first researchers in the world to run scientific applications on an exascale system.

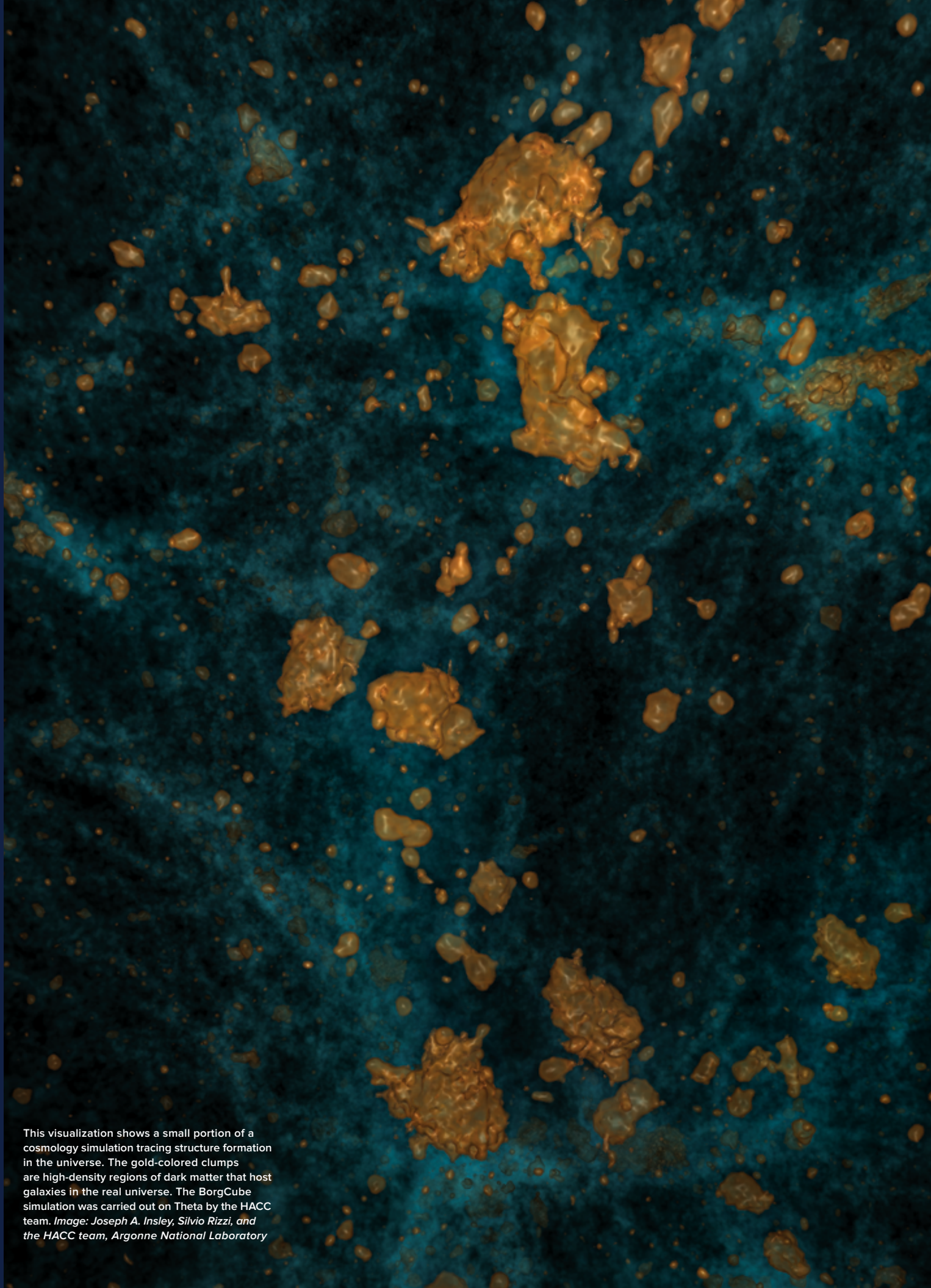
Based on the highly successful ALCF Early Science Programs (ESP) for Mira and Theta, the Aurora ESP is designed to prepare key applications for the architecture and scale of the exascale supercomputer, and solidify libraries and infrastructure to pave the way for production applications to run on the system.

In addition to fostering application readiness for the future supercomputer, the ESP allows researchers to pursue innovative computational science projects not possible on today's leadership-class supercomputers.

Through open calls for proposals, the ALCF has awarded pre-production computing time and resources to 15 projects that will use various simulation, data, and learning techniques. The ESP projects originate from universities and national laboratories across the country and span a wide range of disciplines that cover key scientific areas and numerical methods.

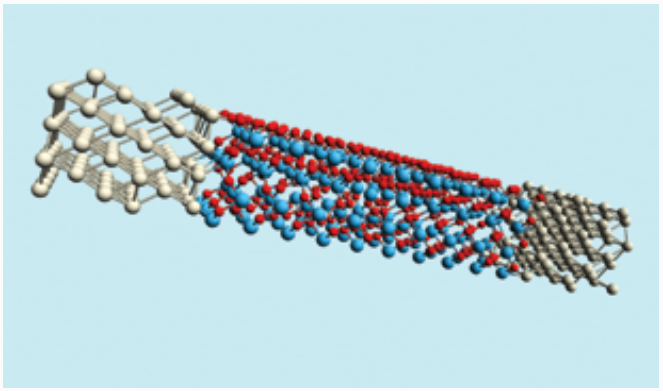
The PI-led project teams consist of core developers of the application, domain science experts, and an ALCF postdoctoral appointee funded for each project. The teams will receive hands-on assistance to port and optimize their applications for the new architecture using systems available today and early Aurora hardware when it is available.

The ALCF will host numerous training events to help the Aurora ESP project teams prepare their codes for the coming system, with assistance from Intel and Cray. The facility will also share technical reports that detail the techniques used by the ESP projects in preparing their applications for the new system.



This visualization shows a small portion of a cosmology simulation tracing structure formation in the universe. The gold-colored clumps are high-density regions of dark matter that host galaxies in the real universe. The BorgCube simulation was carried out on Theta by the HACC team. *Image: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory*

Simulation Projects



Hafnium oxide semiconductor with oxygen vacancies representing the oxygen leakage, inserted between platinum contacts at both ends.
Image: Olle Heinonen, Argonne National Laboratory

SIMULATION

Extending Moore's Law Computing with Quantum Monte Carlo

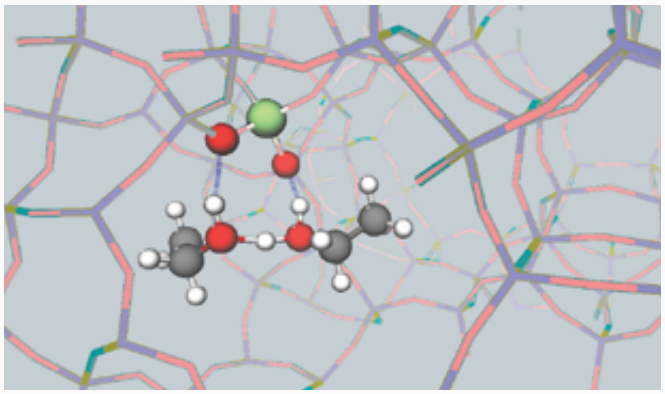
PI Anouar Benali
INST Argonne National Laboratory

This project seeks to identify possible paths forward for extending Moore's Law in silicon complementary metal-oxide-semiconductor (Si-CMOS)-based computing technologies. The researchers will tackle a fundamental materials problem impacting next-generation chips: electrical current leakage through the hafnium oxide-silicon interface. Simulating this problem with the highly accurate quantum Monte Carlo method is only now becoming computationally possible with supercomputers like Aurora.

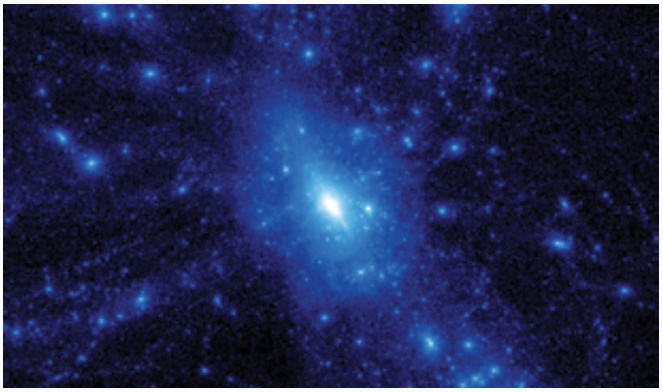
High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang
INST Princeton Plasma Physics Laboratory

The behavior of plasma at the outer edge of a tokamak fusion reactor is critically important to the success of future fusion reactors such as ITER, now under construction in France. With this project, researchers will use the XGC particle-in-cell code to simulate the multiscale behaviors of edge plasma in complex geometries. By advancing the understanding and prediction of plasma confinement at the edge, the team's research will help guide future experimental parameters and accelerate efforts to achieve fusion energy production.



NWChemEx will provide the understanding needed to control molecular processes underlying the production of biomass. *Image: Thom Dunning, Pacific Northwest National Laboratory*



This image shows the dark matter content in a large cluster of galaxies. *Image: JD Emberson and the HACC team, Argonne National Laboratory*

NWChemEx: Tackling Chemical, Materials, and Biochemical Challenges in the Exascale Era

PI Thom Dunning
INST Pacific Northwest National Laboratory

This project seeks to develop a next-generation molecular modeling package that supports chemistry research on Aurora and other exascale systems. The team's science campaign will address two challenges involved in the development of advanced biofuels: the design of feedstock for the efficient production of biomass, and the design of new catalysts for converting biomass-derived chemicals into fuels.

Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann
INST Argonne National Laboratory

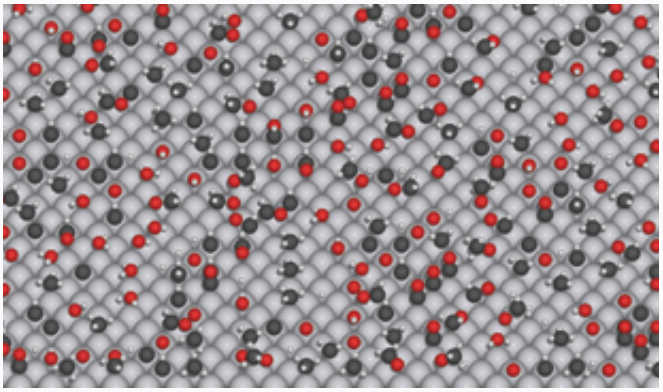
Researchers will use Aurora to carry out cosmological hydrodynamics simulations that cover the enormous length scales characteristic of large sky surveys, while at the same time capturing the relevant small-scale physics. The team will simulate large fractions of the universe, including not only gravity acting on dark matter, but also baryons and gas dynamics using a new, smoothed particle hydrodynamics method. These simulations are deeply coupled with guiding and interpreting observations from present and near-future cosmological surveys.

Extreme-Scale Unstructured Adaptive CFD

PI Kenneth Jansen
INST University of Colorado Boulder

This project seeks to advance simulations in two complex flow regimes: aerodynamic flow control and multiphase flow. The aerodynamic flow control task involves performing simulations of an aircraft's vertical tail rudder at realistic flight conditions, while the multiphase flow task aims to simulate bubbly flows within realistic nuclear reactor geometries at an unprecedented scale. The simulations will help inform the design of next-generation aircrafts and nuclear reactors by providing insights into 3D active flow control at flight scale and reactor heat exchanger flow physics.

Data Projects



Data science techniques will be used in combination with quantum chemistry simulations to explore the otherwise intractable phase space resulting from gas phase molecules on catalyst surfaces to find relevant configurations and the lowest transition states between them. *Image: Eric Hermes, Sandia National Laboratory*

DATA

Exascale Computational Catalysis

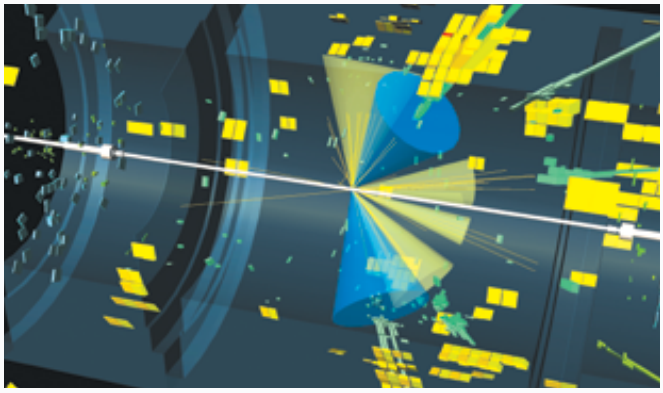
PI David Bross
INST Argonne National Laboratory

Chemical transformation technologies are present in virtually every sector, and their continued advancement requires a molecular-level understanding of underlying chemical processes. This project will facilitate and accelerate the quantitative description of crucial gas-phase and coupled heterogeneous catalyst/gas-phase chemical systems through the development of data-driven tools designed to revolutionize predictive catalysis and address DOE grand challenges.

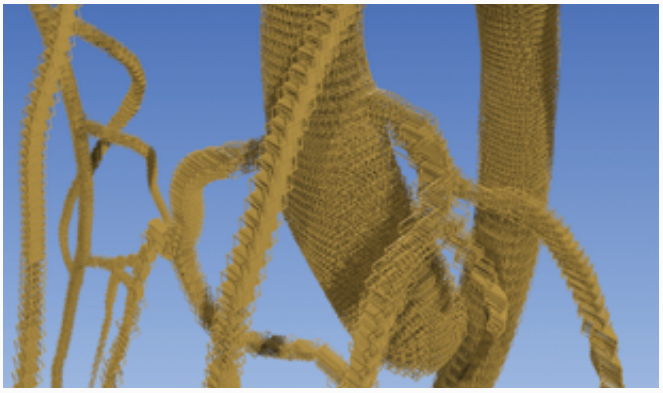
Dark Sky Mining

PI Salman Habib
INST Argonne National Laboratory

This project will connect some of the world's largest and most detailed extreme-scale cosmological simulations with large-scale data obtained from the Large Synoptic Survey Telescope, the most comprehensive observations of the visible sky. By implementing cutting-edge data-intensive and machine learning techniques, it will usher in a new era of cosmological inference targeted at scientific breakthroughs.



A candidate event in which a Higgs boson is produced in conjunction with top and anti-top quarks which decay to jets of particles. The challenge is to identify and reconstruct this type of event in the presence of background processes with similar signatures which are thousands of times more likely.
Image: James Proudfoot, Argonne National Laboratory



Capturing flow in the human aorta requires high-resolution fluid models. In this case, the wireframe boxes indicate each computational bounding box describing the work assigned to an individual task. *Image: Liam Krauss, Lawrence Livermore National Laboratory*

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI Kenneth Jansen
INST University of Colorado Boulder

This project will develop data analytics and machine learning techniques to greatly enhance the value of flow simulations with the extraction of meaningful dynamics information. A hierarchy of turbulence models will be applied to a series of increasingly complex flows before culminating in the first flight-scale design optimization of active flow control on an aircraft's vertical tail.

Simulating and Learning in the ATLAS Detector at the Exascale

PI James Proudfoot
INST Argonne National Laboratory

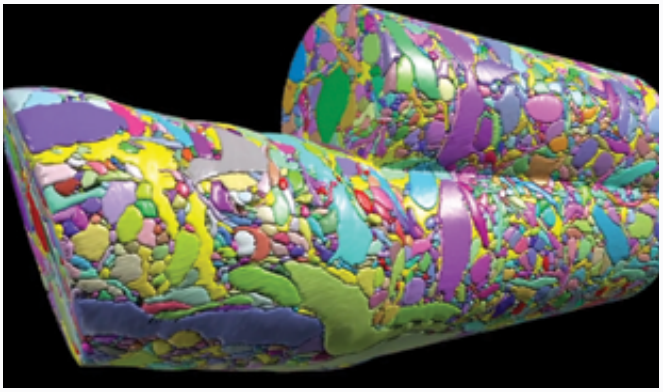
The ATLAS experiment at the Large Hadron Collider measures particles produced in proton-proton collisions as if it were an extraordinarily rapid camera. These measurements led to the discovery of the Higgs boson, but hundreds of petabytes of data still remain unexamined, and the experiment's computational needs will grow by an order of magnitude or more over the next decade. This project deploys necessary workflows and updates algorithms for exascale machines, preparing Aurora for effective use in the search for new physics.

Extreme-Scale In-Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations

PI Amanda Randles
INST Duke University and Oak Ridge National Laboratory

This project advances the use of data science to drive analysis of extreme-scale fluid-structure-interaction simulations so as to develop our understanding of the role biological parameters play in determining tumor cell trajectory in the circulatory system. A cellular-level model of systemic-scale flow represents a critical step towards elucidating the mechanisms driving cancer metastasis.

Learning Projects



To image large brain volumes, individual scanning electron microscope images are registered to form a mosaic. These 2D mosaics are aligned and stacked to form a 3D volume. Analysis is performed to extract sub-volumes corresponding to anatomical structures of interest. *Image: Narayanan "Bobby" Kasthuri, Argonne National Laboratory*

LEARNING

Machine Learning for Lattice Quantum Chromodynamics

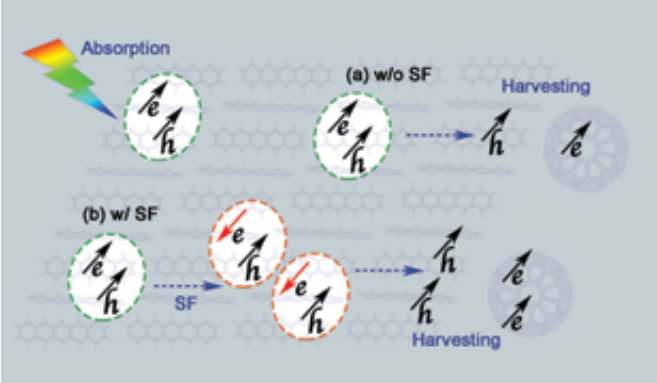
PI William Detmold
INST Massachusetts Institute of Technology

This project will determine possible interactions between nuclei and a large class of dark matter candidate particles. By coupling advanced machine learning and state-of-the-art physics simulations, it will provide critical input for experimental searches aiming to unravel the mysteries of dark matter while simultaneously giving insight into fundamental particle physics.

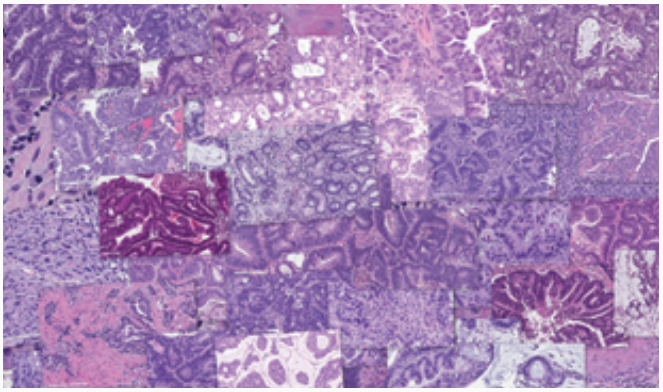
Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI Nicola Ferrier
INST Argonne National Laboratory

This project will develop a computational pipeline for neuroscience that will extract brain-image-derived mappings of neurons and their connections from electron microscope datasets too large for today's most powerful systems. Ultimately the pipeline will be used to analyze an entire cubic centimeter of electron microscopy data.



Schematic of exciton harvesting with and without singlet fission (SF). A singlet exciton (green) is generated when one photon is absorbed. **(A)** Without SF, a singlet exciton only creates one carrier. **(B)** With SF, a singlet exciton converts into two triplet excitons (orange), and there will be double free carriers. *Image: Xiaopeng Wang, Carnegie Mellon University*



Predicting cancer type and drug response using histopathology images from the National Cancer Institute's Patient-Derived Models Repository. *Image: Rick Stevens, Argonne National Laboratory*

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials

PI Noa Marom
INST Carnegie Mellon University

Supercomputers have been guiding materials discovery for the creation of more efficient organic solar cells. By combining quantum-mechanical simulations with machine learning and data science, this project will harness exascale power to revolutionize the process of photovoltaic design and advance physical understanding of singlet fission, the phenomenon whereby one photogenerated singlet exciton is converted into two triplet excitons—increasing the electricity produced.

Virtual Drug Response Prediction

PI Rick Stevens
INST Argonne National Laboratory

Utilizing data frames too large for conventional systems and a deep learning workflow designed to provide new approaches to personalized cancer medicine, this project enables billions of virtual drugs to be screened singly and in numerous combinations, while predicting their effects on tumor cells. The workflow is built from the CANDLE (CANcer Distributed Learning Environment) framework to optimize model hyperparameters and perform billions of inferences to quantify model uncertainty and ultimately deliver results to be tested in pre-clinical experiments.

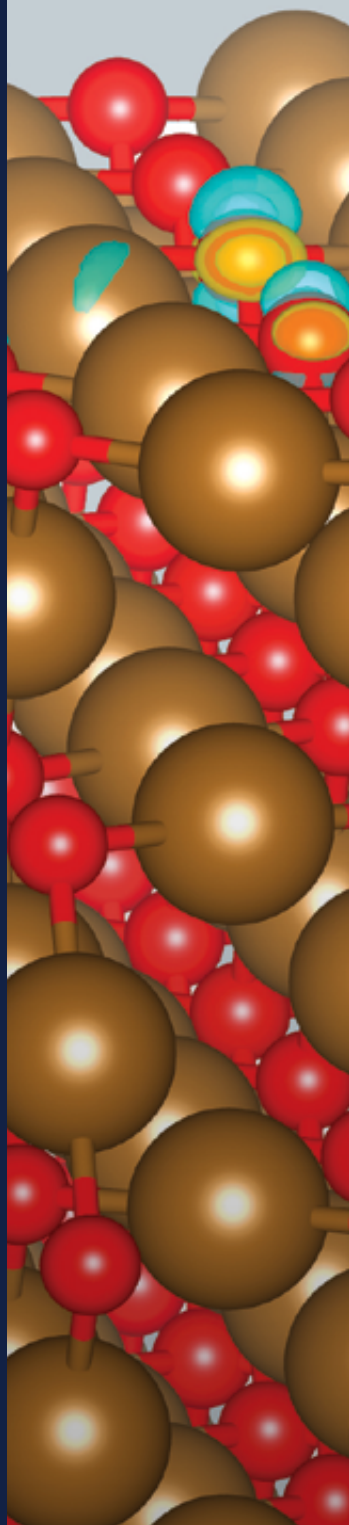
Accelerated Deep Learning Discovery in Fusion Energy Science

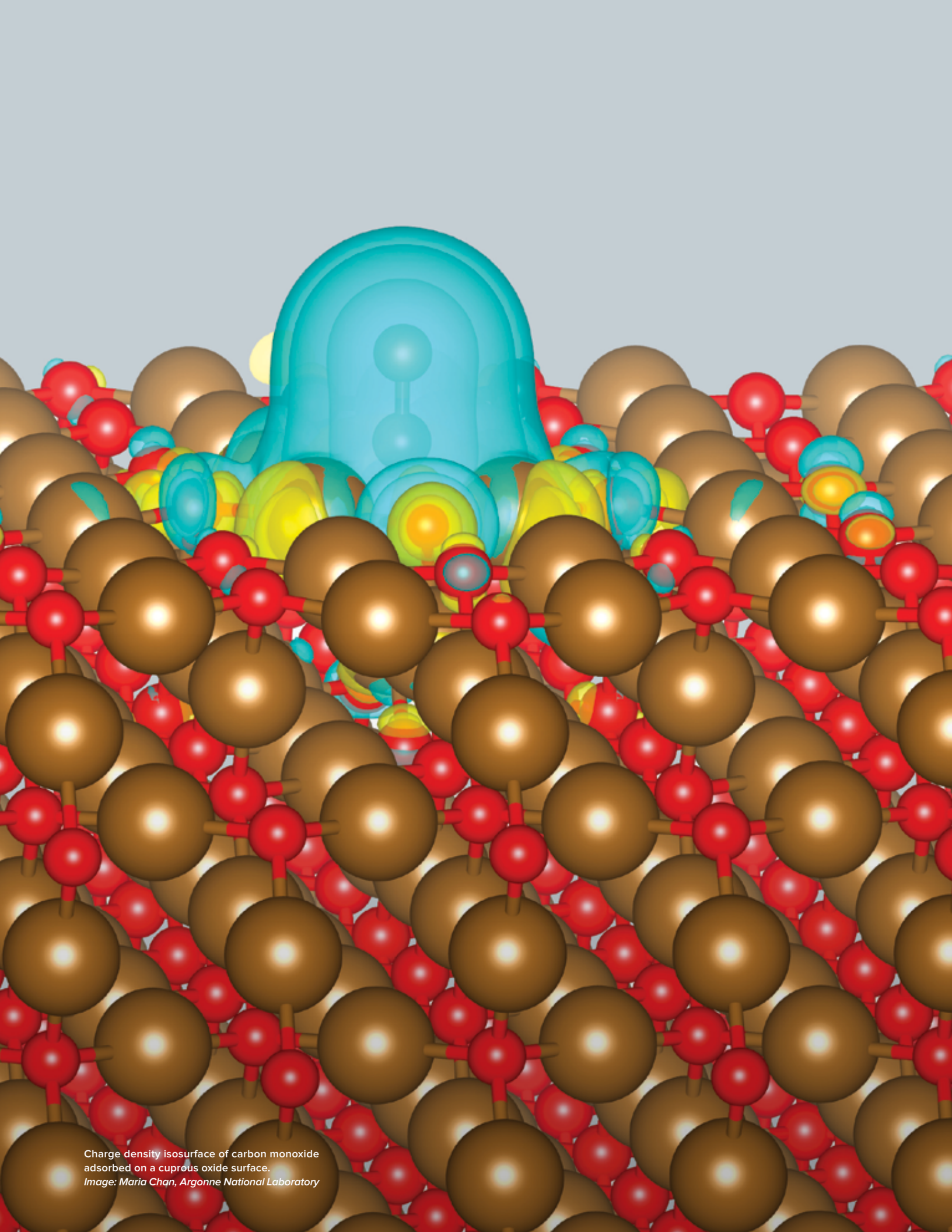
PI William Tang
INST Princeton Plasma Physics Laboratory

Machine learning and artificial intelligence can demonstrably accelerate scientific progress in predictive modeling for grand challenge areas such as the quest for clean energy via fusion power. This project seeks to expand modern convolutional and recurrent neural net software to carry out optimized hyperparameter tuning on exascale supercomputers to make strides toward validated prediction and associated mitigation of large-scale disruptions in burning plasmas such as ITER.

SCIENCE

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





Charge density isosurface of carbon monoxide adsorbed on a cuprous oxide surface.
Image: Maria Chan, Argonne National Laboratory

Accessing ALCF Resources for Science

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

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

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

Application Programs

ADSP

The ALCF Data Science Program (ADSP) supports big data projects that require the scale and performance of leadership computing resources. ADSP projects focus on developing and improving data science techniques that will enable researchers to gain insights into very large datasets produced by experimental, simulation, or observational methods.

ESP

As part of the process of bringing a new supercomputer into production, the ALCF conducts its Early Science Program (ESP) to prepare applications for the architecture and scale of a new system. ESP projects represent a typical system workload at the ALCF and cover key scientific areas and numerical methods.

Allocation Programs

INCITE

The Innovative Novel Computational Impact on Theory and Experiment (INCITE) program aims to accelerate scientific discoveries and technological innovations by awarding ALCF computing time and resources to large-scale, computationally intensive projects that address grand challenges in science and engineering.

ALCC

The ASCR Leadership Computing Challenge (ALCC) program allocates ALCF computing resources to projects that advance the DOE mission, help to broaden the community of researchers capable of using leadership computing resources, and serve the national interests for scientific discovery, technological innovation, and economic competitiveness.

DD

Director's Discretionary (DD) projects are dedicated to leadership computing preparation, INCITE and ALCC scaling, and application performance to maximize scientific application efficiency and productivity on leadership computing platforms.

INCITE/ALCC BY DOMAIN

2018 INCITE allocated hours

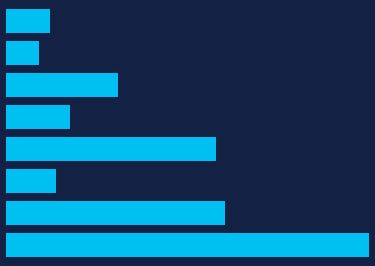
3.78B

Biological Sciences	332	Million Core-Hours
Chemistry	167	
Computer Science	54	
Earth Science	388	
Energy Technologies	115	
Engineering	887	
Materials Science	716	
Physics	1,119	

2018 ALCC allocated hours

1.86B

Biological Sciences	75	Million Core-Hours
Chemistry	56	
Computer Science	190	
Earth Science	109	
Energy Technologies	358	
Engineering	85	
Materials Science	367	
Physics	619	



Note: ALCC data are from calendar year 2018.

Continuing Impact

Supercomputers help accelerate science by providing faster results—but they also generate valuable data that can make the long-term more fruitful.

Leadership-class supercomputers are powerful research tools that can dramatically accelerate scientific discovery. However, some of their benefits require time to emerge. The massive datasets they produce can take many months to analyze. Developing the software necessary to achieve the research goals of large-scale computational science projects can go on for years.

ALCF users therefore frequently seek allocation renewals to continue their work. This allows their research to evolve along with the facility and its increasingly sophisticated computing resources. It also often yields valuable insights.

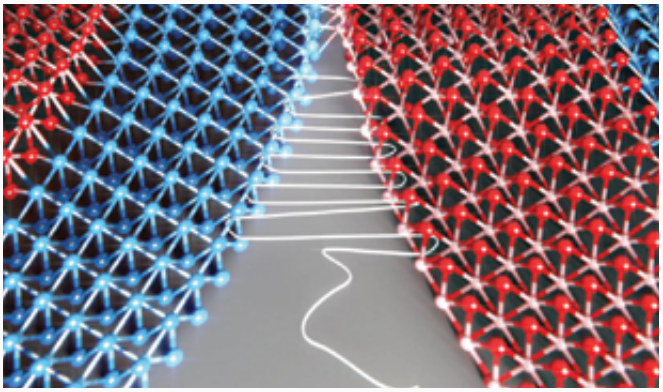
In the following pages, we highlight selected projects that obtained notable results after their allocation year.

Some have highly practical impacts, as seen in the creation of a self-generating, essentially frictionless lubricant and efforts to design more efficient engines. One studied the acoustics of barn owl flight so as to build silent aircraft and wind turbines. Others—such as an investigation into the properties of liquid water that led to functional, atomically "sewn" nano-fabrics—illustrate the rich lifecycle a scientific research project can enjoy as its specialized methods are applied in new and exciting contexts.

Chemistry

Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral Ab Initio Study

PI Robert DiStasio Jr.
INST Cornell University
HOURS ALCC, 175 Million Core-Hours



Researchers sew atomic lattices seamlessly together. *Image: Saien Xie, Cornell University and the University of Chicago*

Merging different crystal structures could lead to the discovery of new materials that bear desirable, highly functional qualities. By applying the same methods they used to accurately characterize the microscopic structures and anomalous density properties of liquid water, researchers from Cornell University and the University of Chicago used ALCF supercomputers to demonstrate that it is possible to fuse materials, atom by atom, for the production of flawless, atomic-scale fabrics. These nano-fabrics have exhibited extraordinary properties, including excellent conductivity and high-efficiency light-emitting diodes.

CHALLENGE After performing highly accurate, large-scale benchmark atomistic simulations of liquid water and aqueous ionic solutions, the researchers redirected their attention to the problem of nano-fabrication as realized through the manipulation of atomic-scale transition metal layers. Realizing the goal of advanced stacking and hetero-integration of 2D heterostructures and superlattices would require materials whose properties can be tuned by the strain necessary for coherent lattice matching.

Such nano-fabrication ("sewing" atom-thick fabrics, for instance) could potentially produce the building blocks for micro-electronic components, but *ab initio* simulations of this process—based in density functional theory—demand massively parallel, leadership-class computing resources.

APPROACH Using the same approach to study weak interactions as they previously did to study liquid water, the researchers ran a series of coarse-grain model simulations that define atomic arrangements and electronic structure calculations to estimate long-range interactions on the surface-deposition of crystal monolayers. WS_2 and WSe_2 served as the transition metal dichalcogenides for the heterostructures and superlattices. ALCF staff members assisted these efforts by helping to create ensemble jobs that run at full capability and by advising the optimization of Mira's nodal computational power.

RESULTS The simulations (in agreement with experimental observation) showed that it is possible to create coherent 2D structures and superlattices a single atom thick for the nanoscale production of electronic devices and which allow for fine-tuning of macroscopic properties including the optical and conductive. Results from this study were published in *Science*.

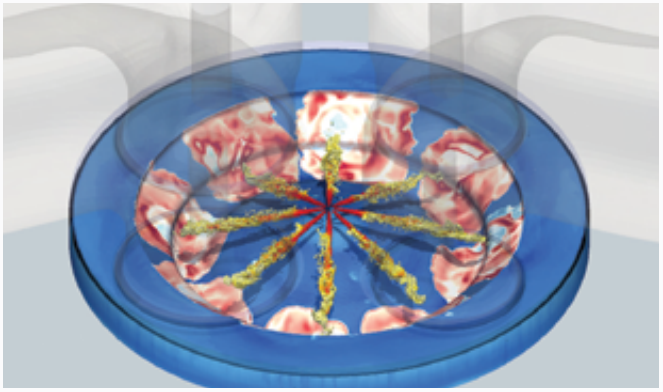
IMPACT Future generations of portable electronics will require both reductions in size and gains in power efficiency. This work has revealed a new path for bringing atomic crystal structures together so as to create efficient, atom-thick conductors with the potential to produce devices that are lighter and consume less than current technologies.

PUBLICATIONS
Xie, S., L. Tu, Y. Han, L. Huang, K. Kang, K. U. Lao, P. Poddar, C. Park, D. A. Muller, R. A. DiStasio Jr., and J. Park. "Coherent, Atomically Thin Transition-Metal Dichalcogenide Superlattices with Engineered Strain," *Science* (March 2018), AAAS.

Engineering

Investigation of a Low-Octane Gasoline Fuel for a Heavy-Duty Diesel Engine

PI Sibendu Som
INST Argonne National Laboratory
HOURS DD, 15 Million Core-Hours



Visualization from a high-fidelity simulation of a heavy-duty engine fueled with a straight-run gasoline performed on the Mira supercomputer by researchers from Argonne National Laboratory, Aramco Research Center–Detroit, and Convergent Science Inc. With more than 100 million cells, this was the largest engine simulation performed to date. *Image: Yuanjiang Pei, Aramco Research Center–Detroit*

Engine modeling and simulation tools have the ability to optimize complex fuel spray and combustion processes for a variety of fuels over a wide range of operating conditions, helping automotive manufacturers improve engine efficiency and performance, while reducing development costs and accelerating time to market. A team of researchers from Argonne National Laboratory and Aramco Research Center–Detroit used ALCF computing resources to advance the design of a heavy-duty diesel engine using a gasoline-like fuel for improved efficiency and performance.

CHALLENGE Traditional engine design simulations in industry are performed on smaller computing clusters with a limited design space that can take months to complete. With access to ALCF supercomputers, researchers can run many engine design scenarios concurrently, allowing them to explore a larger design and parameter space much more quickly.

APPROACH Running the CONVERGE code on Mira, the team performed a first-of-its-kind study using a high-fidelity simulation approach to optimize the fuel spray and combustion bowl geometry on a supercomputer. Model predictions were validated against experimental results generated using the production engine hardware. In an earlier project with Convergent Science, Inc., ALCF staff helped to optimize the company's CONVERGE code on Mira, resulting in a 100x speedup in I/O, an 8x improvement in load balance, and a 3.4x improvement in time-to-solution.

RESULTS The team used Mira to simulate about 2,000 high-fidelity engine design combinations in a matter of days, covering four different operating conditions, six bowl geometries, multiple fuel injector-related configurations, and various start-of-injection scenarios. The team's simulations revealed design scenarios that showed an improvement in fuel efficiency of up to 4.1 percent while maintaining nitrogen oxide emissions within production levels. The computational study allowed the team to narrow down the best-performing scenarios to two specific sets of piston and injector designs for further evaluation.

IMPACT By accelerating the simulation time of various engine scenarios, researchers were able to evaluate an unprecedented number of design variations within a short time span and improve the production design of an engine using a new fuel. Ultimately, the development of novel engine modeling capabilities for supercomputers can help automotive manufacturers advance efforts to improve the fuel economy of vehicles, thereby reducing U.S. dependence on foreign oil and reducing emissions.

PUBLICATIONS

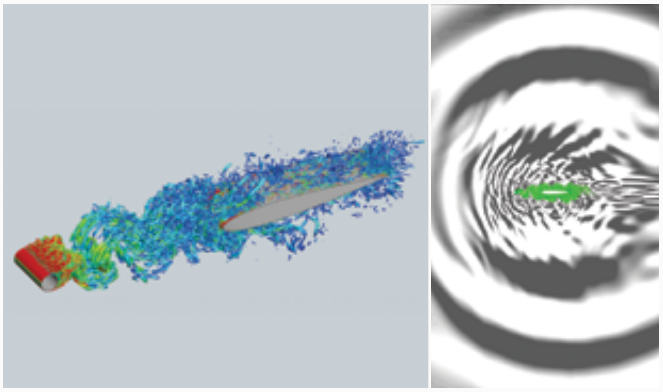
Pei, Y., Y. Zhang, P. Kumar, M. Traver, D. Cleary, M. Ameen, S. Som, D. Probst, T. Burton, E. Pomraning, and P.K. Senecal. "CFD-Guided Heavy Duty Mixing-Controlled Combustion System Optimization with a Gasoline-Like Fuel," *SAE International Journal of Commercial Vehicles* (March 2017).

Pal, P., D. Probst, Y. Pei, Y. Zhang, M. Traver, D. Cleary, and S. Som. "Numerical Investigation of Gasoline-like Fuel in a Heavy-Duty Compression Ignition Engine Using Global Sensitivity Analysis," *SAE International Journal of Fuels and Lubricants* (March 2017).

Engineering

Unraveling Silent Owl Flight to Develop Ultra-Quiet Energy Conversion Machines

PI Anupam Sharma
INST Iowa State University
HOURS ALCC, 25 Million Core-Hours



Simulation results from the team's computational framework: **(A)** an investigation of a blade geometry with serrations inspired by the leading-edge comb of the owl and **(B)** a visualization of the radiated sound field for a model problem. *Image: Anupam Sharma, Iowa State University*

The night owl is known for its acoustic stealth in flight, but the physical mechanisms that enable its silent movement are not yet clearly understood. This ALCC project uses high-resolution computational fluid dynamics simulations of wind turbine blade geometries inspired by the owl plumage to fill this gap in our understanding. The results will help in designing and developing low-noise wind turbines, aircraft engines, and other engineering devices.

CHALLENGE Acoustic emission (noise) from wind turbines is curtailing the growth of wind energy—currently the primary renewable energy source in the U.S. and in the world. A majority of the noise radiated from wind turbines is generated by the interaction of wind with blade surfaces. One remedy may come by studying the night owl, which is known for its silent flight. Previous investigations have demonstrated that there are three unique feather features responsible for the owl's acoustic stealth, but scientists don't yet know the physical mechanisms behind it.

APPROACH In this ALCC project, researchers used Mira to carry out a systematic numerical investigation of the unique owl feather features. High-fidelity numerical simulations offered extremely high spatial and temporal resolution that enabled source diagnostics to identify how the feather features curb noise generation. The simulations used a well-established high-order accurate flow solver, FDL3DI, and an in-house acoustics solver. They investigated several owl-inspired geometries that were idealized representations of the unique feather features. Mira enabled wall-resolved large eddy simulations of such geometries for the first time.

RESULTS The team was able to show that noise was reduced by 5 decibels with serrated leading edge and 10 decibels with finlets. These findings, alongside the physical mechanisms that cause them, were recently published in the *International Journal of Aeroacoustics*. The results will be combined with ongoing experimental measurements at Virginia Tech to allow a comprehensive understanding of silent owl flight.

IMPACT Noise is a significant issue for many industry applications, including wind turbines, aircraft engines, and combustion turbines used for electricity generation, cooling fans, and ventilation systems. The knowledge and understanding gained from these simulations can provide a transformative jump towards developing nearly silent energy conversion machines.

PUBLICATIONS

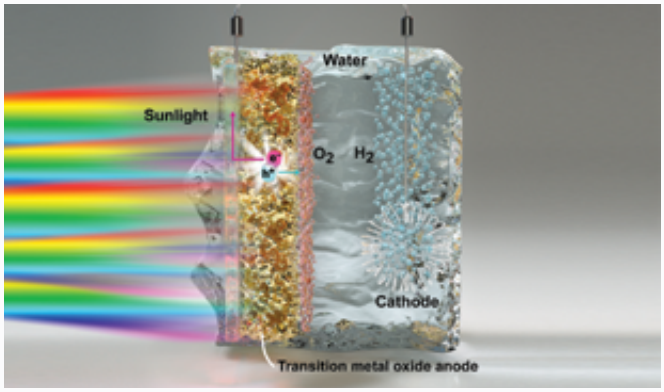
Agrawal, B. R. and A. Sharma. "Numerical Analysis of Aerodynamic Noise Mitigation via Leading Edge Serrations for a Rod-Airfoil Configuration," *International Journal of Aeroacoustics* (September 2016), SAGE Publications.

Bodling, A., B. R. Agrawal, A. Sharma, I. Clark, W. N. Alexander, and W. Devenport. "Numerical Investigations of Bio-Inspired Blade Designs to Reduce Broadband Noise in Aircraft Engines and Wind Turbines," *55th AIAA Aerospace Sciences Meeting* (June 2017).

Materials Science

First-Principles Simulations of Functional Materials for Energy Conversion

PI Giulia Galli
INST Argonne National Laboratory
The University of Chicago
HOURS Theta ESP, 50 Million Core-Hours



Schematic representation of a photoelectrochemical cell, highlighting the photoanode surface/water interface. *Image: Peter Allen, The University of Chicago*

The application of advanced theoretical methods can improve property predictions and thereby accelerate the discovery of materials for use in devices that convert solar and thermal energy. Argonne National Laboratory and University of Chicago researchers are therefore using ALCF supercomputing resources to investigate the properties of nanostructured materials that can facilitate the creation of future, highly optimized devices.

CHALLENGE This project aims to predict the electronic and thermal properties of materials exhibiting complex structures on multiple length scales, with a particular focus on the opto-electronic properties of inorganic nanostructured samples for use in solar cells that exploit intermediate band transitions and/or multi-exciton generation for carrier multiplication.

The researchers here homed in on WO_3 (a promising anode for photo-electrochemical cells) with a finite-temperature study completed by coupling first principles molecular dynamics simulations with many-body perturbation theory.

APPROACH *Ab initio* molecular dynamics simulations computed the ensemble averages of thermodynamic and transport properties of complexly nanostructured materials. These same atomistic trajectories subsequently served as the input for many-body perturbation theory calculations to compute electronic properties (including band gaps, band edges, absorption spectra, and dielectric properties). Using Theta, the researchers performed spin-polarized density functional theory calculations implemented in Qbox and Quantum ESPRESSO. Qbox also enabled the calculation of first principles molecular dynamics trajectories from which configurations were sampled to compute quasiparticle corrections using the WEST code. Coordinating with ALCF staff yielded significantly improved single-node performance (exploiting Theta's architecture) and parallel scalability of Qbox and WEST.

RESULTS The researchers identified the properties of WO_3 surfaces crucial to understanding and predicting the material's reactivity when in contact with water (including excess charges brought about by defects and their dynamics in solvated environments), and proposed a mechanism for the formation of reactive radical groups at the interface with water. The study showed that the optimization of oxide photo-absorbers for water catalysis requires realistic surface models that include oxygen vacancies (the most common defects present in these materials). It also revealed the high level of electronic structure theory necessary for good simulative agreement with photoemission experiments.

IMPACT This work—with unprecedented accuracy—optimizes the properties of materials to be used for solar and thermal energy conversion. This furthers the Materials Genome Initiative by providing truly predictive tools for device performance.

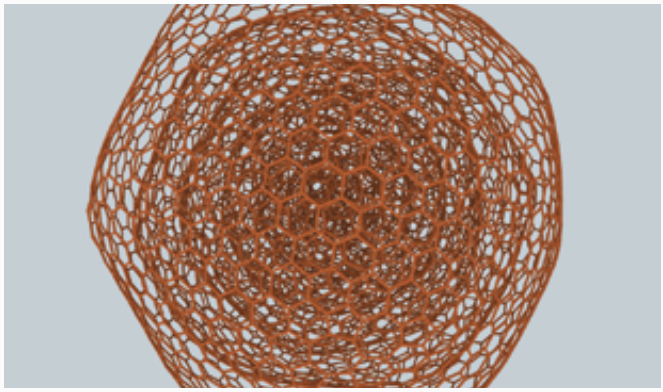
PUBLICATIONS

Gerosa, M., F. Gygi, M. Govoni, and G. Galli. "The Role of Defects and Excess Surface Charges at Finite Temperature for Optimizing Oxide Photoabsorbers" *Nature Materials* (accepted), Springer Nature.

Materials Science

Reactive Mesoscale Simulations of Tribological Interfaces

PI Subramanian Sankaranarayanan
INST Argonne National Laboratory
HOURS INCITE, 40 Million Core-Hours



Atomistic simulations indicate that both silicon and molybdenum induce structural degradation of nanodiamonds: silicon induces rapid amorphization of the diamond lattice and the amorphous carbon subsequently transforms into carbon onions (pictured) which lead to a near frictionless state. *Image: Badri Narayanan and Subramanian Sankaranarayanan, Argonne National Laboratory*

Superlubricity—a state in which friction essentially disappears—is a highly desirable property for automobiles and countless other mechanical assemblies that lose efficiency and wear down due to friction, but achieving this at the macroscale remains a major challenge. Superlubric materials could help reduce fuel needed to overcome friction in automobiles, improve efficiency and lifetime of mechanical components, and lower the undesired environmental impacts from oil-based lubricants. In this INCITE project, a team of researchers used Mira to develop a new material that demonstrates superlubricity in dry environments.

CHALLENGE It is estimated that nearly one-third of the fuel used in automobiles is spent to overcome friction. Oil-based lubrication is the conventional approach to reducing friction and wear in the automotive industry, but the oil waste leads to adverse environmental impacts. The use of two-dimensional materials such as graphene as a lubricant has recently become promising, but it is poorly understood how stress-induced reactions at the sliding interface during relative movement form byproducts in an oil-free environment.

APPROACH In 2015, a multidisciplinary team from Argonne created a novel material that demonstrated superlubricity at the macroscale for the first time. To further develop this lubricant technology, the researchers explored the impact of using the two-dimensional material molybdenum disulfide. The researchers coupled laboratory experiments at Argonne's Tribology Laboratory and Center for Nanoscale Materials with large-scale simulations performed at the ALCF to inform the design of the material. To enable the computationally demanding reactive molecular dynamics simulations, ALCF staff collaborated with IBM, Lawrence Berkeley National Laboratory, and Sandia National Laboratories to optimize the performance of LAMMPS for Mira and other many-core architectures.

RESULTS The team's large-scale atomistic simulations revealed molecular insights into a mechanical stress-induced tribochemical reaction that led to superlubricity. They found that the molybdenum disulfide was breaking up into molybdenum and sulfur and reacting with the nanodiamonds to convert them into onion-like carbon structures, which can be used as a dry lubricant. The team published their findings in *Nature Communications*.

IMPACT This new self-generating lubricant lasts longer than traditional dry lubricants. Its potential applications include wind turbine gears, magnetic disc drives in computers, and mechanical rotating seals for microelectromechanical and nanoelectromechanical systems.

PUBLICATIONS

Berman, D., B. Narayanan, M. J. Cherukara, S. K. R. S. Sankaranarayanan, A. Erdemir, A. Zinovev, and A. V. Sumant. "Operando Tribochemical Formation of Onion-Like-Carbon Leads to Macroscale Superlubricity," *Nature Communications* (March 2018), Springer Nature.

2018 Science Highlights

The ALCF user community accelerates scientific discovery across disciplines, advancing our knowledge of the universe at all scales.

With hundreds of thousands of processors working in parallel, supercomputers allow users to achieve scientific breakthroughs that would not otherwise be possible. From detailed atomic-level simulations to massive cosmological studies, researchers can investigate extremely complex physical systems and processes that are too small or large, costly, or dangerous to study in a laboratory.

Each year, ALCF users produce impressive results, whether it be developing and demonstrating novel computational methods or publishing papers in high-impact scientific journals.

In the following pages, we present a selection of notable results from current projects supported by the ALCF's various allocation programs.

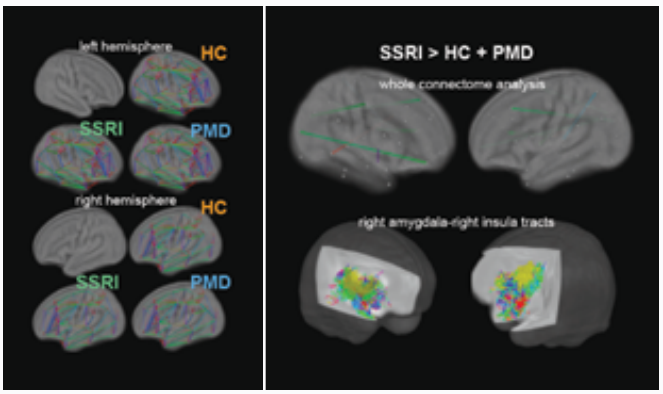
Among this year's highlights is a project that is using advanced data mining techniques to pinpoint promising solar cell materials for synthesis and subsequent experimental studies. Another project is performing high-precision nuclear physics calculations to shed light on how subatomic matter organizes itself.

You will also read about a company using ALCF systems to accelerate its efforts to develop commercially viable fusion energy; a research team simulating complex turbulent conditions at an unprecedented level of detail to inform the design of improved aircraft tails and rudders; and several other projects pursuing breakthroughs in both basic and applied research in fields ranging from biology and chemistry to particle physics and computer science.

Biological Sciences

Developmental Trajectory of Brain and Cognition in Youth in Physiological and Pathological Conditions

PI Jiook Cha
INST Columbia University
HOURS DD, 5 Million Core-Hours



(A) Estimate white matter connections in each group (HC-healthy controls, SSRI-infants exposed to SSRI, PMD-infants exposed to maternal depression but not to SSRI). **(B)** Increase in white matter connectivity in SSRI-exposed infants. *Image: American Medical Association*

For a number of brain diseases, researchers have yet to determine clinically useful markers or targets for diagnosis and therapeutics. The advent of rigorous computational data analytics has yielded brain imaging studies that display the potential of throughput imaging analysis as a diagnostic tool. A team of Columbia University researchers is using ALCF computing resources to conduct a data-driven brain analysis to make predictions of normal or pathological conditions.

CHALLENGE This project aims to determine novel brain imaging markers for psychiatric disorders in youth, using high-throughput brain phenotyping and machine learning. Doing so will allow estimation of complex morphometry and connectomes of thousands of brains (utilizing data collected by the National Institute of Health), and the use of endophenotypes to make clinical predictions. The researchers have specifically sought to determine whether prenatal exposure to selective serotonin reuptake inhibitors (SSRIs) is associated with fetal brain development.

APPROACH This work will be completed via assessment of white matter fibers and scalable deep learning algorithms for predictive modeling. Brain imaging analysis will be performed through established pipelines for volumetric and connectomic estimation at the individual level. Deep learning will be applied to predict the risk for psychiatric illnesses. The researchers have been extensively testing the codes Freesurfer and Mrtrix3, both of which are designed for high-throughput brain magnetic resonance imaging analysis.

RESULTS Assessing a sample of 98 mother/infant dyads, brain scans indicated significant gray matter expansion in the right amygdala of SSRI-exposed infants compared against both healthy controls and infants exposed to untreated maternal depression. Additionally, connectome-level analysis of white matter structural connectivity showed the SSRI-exposed group experienced a significant increase in connectivity between the right amygdala and right insula. These findings suggest that prenatal exposure to SSRIs affects regions critical to emotional processing. Overall, the study highlights the need for further research on the potential long-term behavioral and psychological outcomes of these neurodevelopmental changes.

IMPACT This work will generate essential data for the largest-ever brain imaging study in child psychiatry and developmental neuroscience. Present accomplishments will permit the construction of a highly scalable deep learning algorithm with which to derive rich information concerning the brain's health status for predictive modeling, and contribute to the development of early, affordable, and non-invasive detection of psychiatric diseases.

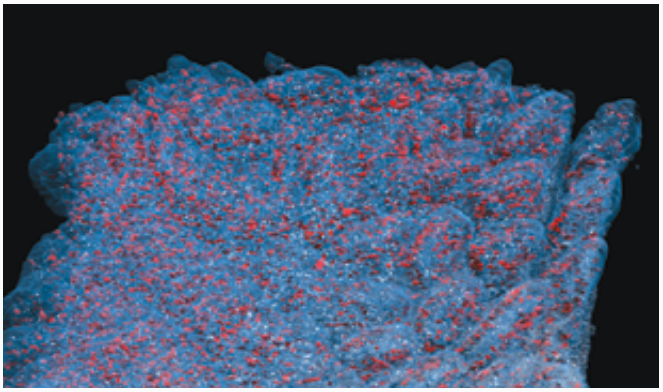
PUBLICATIONS

Lugo-Candelas, C., J. Cha, S. Hong, V. Bastidas, M. Weissman, W. P. Fifer, M. Myers, A. Talati, R. Bansal, B. S. Peterson, C. Monk, J. A. Gingrich, and J. Posner. "Associations Between Brain Structure and Connectivity in Infants and Exposure to Selective Serotonin Reuptake Inhibitors During Pregnancy," *JAMA Pediatrics* (June 2018), American Medical Association.

Biological Sciences

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

PI Doga Gursoy
INST Argonne National Laboratory
HOURS ADSP, 25 Million Core-Hours



Reconstruction of the mouse enteric nervous system. Blue regions are tissue and red are microbiota. *Image: Doga Gursoy, Argonne National Laboratory*

Brain maps that detail the interconnections between billions of neurons ("connectomes") have the potential to revolutionize our understanding of neural computation and disease. Given that connectomes contain massive amounts of data, large-scale computational infrastructures are required for their interpretation. As such, Argonne researchers are developing through the ALCF Data Science Program a computational pipeline that will facilitate intricate, deep-level mappings of brain function.

CHALLENGE Several national and international efforts —including one at Argonne's Advanced Photon Source—are underway to collect the petabytes (and, eventually, exabytes) of image data necessary to map brains using nanometer-resolution serial-section electron microscopy and micron-resolution synchroton-based X-ray microscopy. The large-scale data and computational pipeline Argonne researchers are developing to manage the resultant data must integrate exascale approaches for understanding brain structure and pathology, and address the challenges of data reconstruction, segmentation, and analysis.

APPROACH The researchers have constructed the Python-based pipeline Flexible Learning-Free Segmentation and Reconstruction of Neural Circuits (FLoRIN) and are developing a hyperparameter optimizer called SHADHO. FLoRIN sidesteps machine learning and deep learning, instead utilizing modernized approaches to classical, deterministic computer vision techniques so as to overcome the problem of training-data acquisition. FLoRIN operates by computing a grid of neural image stack subvolumes for parallel processing. Subvolumes are then partitioned among nodes singly, with a grid of sub-subvolumes subsequently computed for each nodal core to process in parallel. Segmentation of these sub-subvolumes can now proceed before their recombination into a single volume. Connected components within the segmentation are then identified and geometrically grouped. SHADHO, meanwhile, attempts to increase the throughput of a hyperparameter search to adjust scheduling and send models to the appropriate hardware.

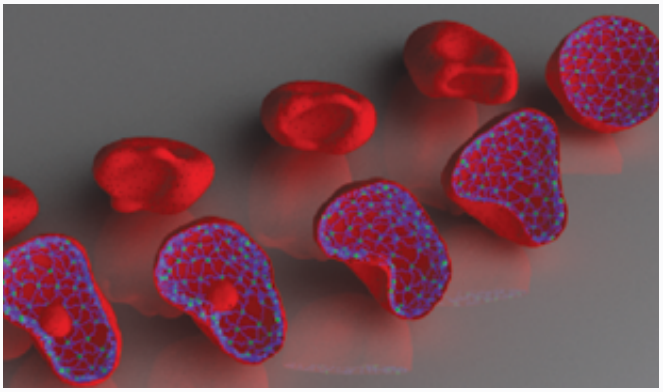
RESULTS The researchers deployed FLoRIN on Theta and successfully developed a method for automatically setting FLoRIN parameters using proxy data. Moreover, FLoRIN is being applied to the co-registration problem, allowing multiple images to be studied in series so as to identify neural changes: one imaged neural volume is automatically mapped to another via estimated transformation matrices.

IMPACT The realization of an exascale data and computational pipeline for neuroscience will revolutionize our understanding of brain function and pathology. Connectomics can help elucidate how even the smallest neurological changes contribute to diseases and disorders such as Alzheimer's and autism, perhaps thereby providing a path to improved treatments.

Biological Sciences

Multiscale Simulations of Hematological Disorders

PI George Karniadakis
INST Brown University
HOURS ALCC, 46 Million Core-Hours
(ALCF: 20M; OLCF: 26M)



Simulations of vesiculation and endocytosis of reticulocytes (young red blood cells) in hereditary spherocytosis. *Image: He Li and Lu Lu, Brown University*

Researchers from Brown University are using computational modeling powered by ALCF supercomputers to simulate the biological processes that cause the alterations of red blood cells (RBCs) in sickle cell anemia, hereditary spherocytosis, and hereditary elliptocytosis. The obtained simulation results improve our understanding of the pathogenesis of these hematological disorders. The developed computational framework can help physicians to make disease prognoses.

CHALLENGE The underlying mechanisms that alter the biomechanics and morphologies of RBCs at different organs in hematological disorders are not fully understood because of the limitations of laboratory approaches. Computational modeling can serve as an important complement to elucidate these complex processes. Researchers at Brown University intend to develop multiscale models to elucidate the mechanics of RBC alterations in the spleen and dissect the pathogenic role of spleen in hematological disorders.

APPROACH The mechanics of diseased RBCs passing through the splenic inter-endothelial slit (IES) were simulated by OpenRBC (developed at Brown University), a high-performance computational simulator of RBCs which simulates an entire RBC by using some 4 million coarse-grained particles.

RESULTS As described in their publication in the *Proceedings of the National Academy of Sciences* the team discovered that hereditary spherocytosis RBCs lose surface area through shedding vesicles during their passage through IES due to the weakened cohesion between the cytoskeleton and the lipid bilayer. Loss of surface area from hereditary spherocytosis RBCs becomes more pronounced as the degree of protein deficiency is elevated. In hereditary elliptocytosis, RBCs are elongated after traversing IES, contributing to the shape transition to elliptical shapes. In severe forms of hereditary elliptocytosis, RBCs break into fragments during their passage of IES.

IMPACT The multiscale simulations performed in this project provide a new "incendiary firefighter" paradigm for the role of spleen in hematological disorders. The spleen not only senses and clears RBCs with abnormal shapes and deformability, but also contributes to pathological alternations of RBCs in blood disorders. The framework established in this projected is sufficiently general to be extended to elucidate the pathophysiological roles of the spleen in other blood diseases.

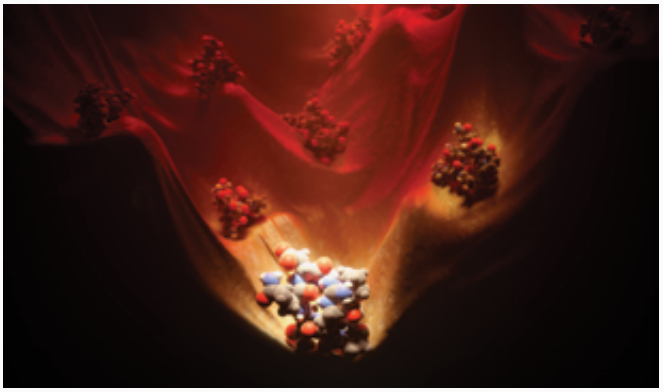
PUBLICATIONS

Li, H., L. Lu, X. Li, P. A. Buffet, M. Dao, G. E. Karniadakis, and S. Suresh. "Mechanics of Diseased Red Blood Cells in Human Spleen and Consequences for Hereditary Blood Disorders," *Proceedings of the National Academy of Sciences* (September 2018).

Chemistry

Advancing Design and Structure Prediction of Proteins and Peptides

PI David Baker
INST University of Washington
HOURS INCITE, 120 Million Core-Hours



An artist's conception of the power of computational design to explore and illuminate structured peptides across the vast energy landscape *Image: Vikram Mulligan, University of Washington*

Proteins are complex molecules that drive virtually all cellular functions in living organisms. Using ALCF supercomputers, researchers from the University of Washington are advancing protein structure modeling capabilities to enable the design of novel chains of amino acids (peptides) for the treatment of a host of diseases and medical conditions. This capability could significantly reduce the costs associated with drug design and discovery research.

CHALLENGE As with the design of a protein, integral to the design of a peptide drug is creating a molecule with a rigid structure that perfectly complements the shape and charge of a binding pocket in a target site. However, for several reasons, peptide design is a more challenging task than protein design. For example, synthetic peptides may lack regular secondary structures or hydrophobic cores and can contain local structures inaccessible to left-handed amino acids, creating computationally expensive hurdles.

APPROACH Researchers employed Mira to enumerate the stable structures that macrocyclic peptides composed of left- and right-handed amino acids can adopt. Sequence design and energy calculations followed near-exhaustive backbone sampling.

Rosetta, the code used for protein structure prediction and design, traditionally scales poorly. The researchers worked to improve this deficit by enabling support for multiple servers to create and delegate tasks, which, in principle, will allow Rosetta to scale to the whole of Mira.

RESULTS As detailed in *Science*, to enable the design of cyclic peptides which fold into well-defined shapes with specific targets, the researchers have developed a general energy function in Rosetta demonstrated to increase modeling accuracy for a wide range of molecules; it will soon be applicable to non-canonical amino acids. For energy optimization, a genetic algorithm was integrated with the energy function, greatly augmenting the code's flexibility and improving its efficiency by a factor of up to 1,000.

Energy minima in alanine dipeptide were subsequently evaluated, with results to be published in the *Journal of Computational Chemistry*.

IMPACT Improving the code used for structure design and prediction can dramatically lower the costs of drug creation and broadly impacts simulation-based material science. The advancements automate design work previously dependent on human intuition, while augmenting the code's ability to handle broader arrays of building blocks and therapeutic targets. Some of the peptides studied could eventually rank among the most potent therapeutics identified.

PUBLICATIONS

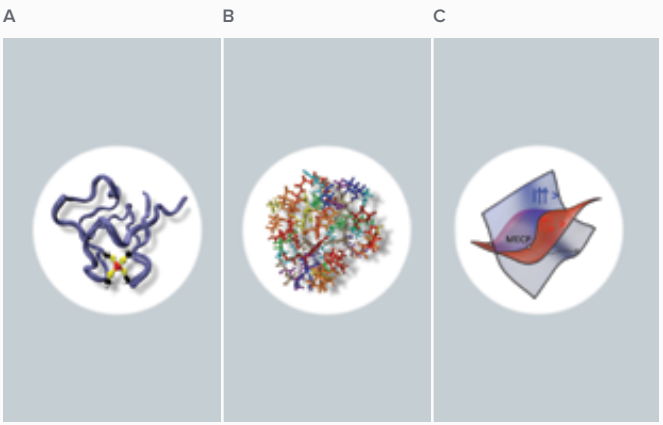
Hosseinzadeh, P., G. Bhardwaj, V. Mulligan, M. Shortridge, T. Craven, F. Pardo-Avila, S. Rettie, D. Kim, D. Silva, Y. Ibrahim, I. Webb, J. Cort, J. Adkins, G. Varani, and D. Baker. "Comprehensive Computational Design of Ordered Peptide Macrocyles," *Science* (December 2017), AAAS.

Mironov, V., Y. Alexeev, V. Mulligan, and D. Fedorov. "A Systematic Study of Minima in Alanine Dipeptide," *Journal of Computational Chemistry* (accepted), John Wiley & Sons.

Chemistry

Spin-Forbidden Catalysis on Metal-Sulfur Proteins

PI Sergey Varganov
INST University of Nevada, Reno
HOURS ALCC, 42 Million Core-Hours



(A) Protein rubredoxin, **(B)** fragment molecular orbital model, **(C)** intersection of potential energy surfaces with different electronic spin multiplicities *Image: Danil S. Kaliain, Purdue University and University of Nevada, Reno*

In many energy- and technology-related applications, chemical reactions are impractically slow and require catalysts, ingredients that accelerate the reaction rate. Researchers from the University of Nevada, Reno are using ALCF computing resources to study the transition metal-based catalysts often used in biological systems, this work being a major step toward the development of future industrial catalysts.

CHALLENGE By investigating the mechanisms of catalytic reactions on metal-sulfur proteins (emphasizing hydrogen oxidation/reduction on rubredoxin proteins and NiFe hydrogenase), the researchers expect to gain insight into the catalyses of biological systems and contribute to the design of future catalysts—a DOE Grand Challenge—based on inexpensive and earth-abundant first-row transition metals. Given the thousands of atoms involved in the systems' proteins, modeling hydrogen oxidation/reduction reactions requires the leadership-class systems at ALCF.

APPROACH The researchers are using Mira to run the General Atomic and Molecular Structure System (GAMESS) quantum chemical package with the novel fragment molecular orbital (FMO) minimum crossing point search module that they developed. GAMESS is largely based on Fortran 77 with parts written in Fortran 90 and C, and parallelization achieved via MPI. FMO is being used in combination with density functional theory (DFT) to optimize the equilibrium structures, transition states, and minimal energy crossing points (MECP) between electronic states with different spin multiplicities for the hydrogen oxidation/reduction reactions on the metal-sulfur proteins and similar selenoproteins. The obtained structures are used to calculate the rates of hydrogen oxidation and reduction, providing fundamental insight into the mechanisms of metalloenzymatic catalysis, including understanding of the importance of nonadiabatic transitions and specific residues in the active site environment.

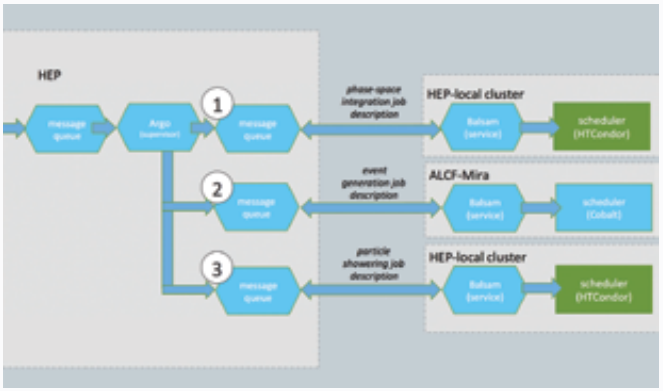
RESULTS The researchers have shifted their focus to production runs, including fully quantum calculations on rubredoxin using FMO. They achieved convergence of the self-consistent FMO DFT method and obtained a good scalability of the equilibrium and MECP geometry calculations, which are nearly optimized. They executed MECP search calculations, as well as geometry optimization runs on quartet and sextet electronic spin states of solvated rubredoxin, allowing prediction of spin-forbidden transition rates with and without bound hydrogen molecules.

IMPACT This project aims to tackle a DOE's Grand Challenge: understanding mechanisms and dynamics of catalyzed reactions. Understanding how transition metal-based catalysts function and how their analogs can be made to work outside fragile biological systems represents a major step toward developing future cost-saving industrial catalysts—on which 95 percent of chemical production depends.

Computer Science

Balsam: Workflow Manager and Edge Service for HPC Systems

PI Thomas Uram, Taylor Childers
INST Argonne National Laboratory
HOURS ALCC/DD, 150+ Million Core-Hours



A schematic of the ATLAS deployment of Balsam on multiple computing resources to execute a workflow with alternating serial and parallel stage. *Image: Thomas Uram, Argonne National Laboratory*

The ALCF's Balsam tool was originally developed as an "edge service," providing a simple, adaptable interface between HPC facilities and the job management systems operated by large-scale experimental science projects. ALCF researchers have further developed Balsam to serve as a workflow management tool that manages large-scale job campaigns for users, while diminishing the burden on the user and opening opportunities for optimizing how these jobs are submitted and executed.

CHALLENGE Integrating leadership computing facilities into the workflows of large-scale experiments, such as CERN's Large Hadron Collider (LHC), requires solving several technical challenges, including authentication, interfacing with schedulers to submit jobs, managing input and output data transfers, and monitoring running jobs. Many users of the facility face similar challenges when configuring and submitting collections of hundreds or thousands of jobs, handling errors and resubmitting, and tracking job metadata, progress and output files.

APPROACH The goals of Balsam were twofold: to integrate ALCF supercomputers with the production system of the LHC's ATLAS experiment, and to build a modular system that could be easily adapted to the needs of other projects and diverse supercomputers. It was designed to enable users to easily add jobs to a job database, from which Balsam subsequently executes jobs according to queue policies, queue depth, job dependencies, and user preferences, with little to no user intervention. Job dependency graphs are persistent, which means they can be extended while jobs are running or after they have finished, to capture all details of a complex workflow even if it was not initially fully specified; this is useful for provenance and scientific reproducibility.

RESULTS The ALCF/ATLAS project has used Balsam to run hundreds of millions of compute hours of event generation jobs on ALCF systems. The research team also used Balsam for production science at the National Energy Research Scientific Computing Center (NERSC), demonstrating Balsam's portability and efficacy.

More recently, the ALCF has released Balsam publicly to help researchers handle the cumbersome process of running many jobs across one or more HPC resources. In addition, the ALCF team has used Balsam in studies of hyperparameter optimization in deep learning (DeepHyper) and in quantum chemistry applications, both running ensemble jobs on more than 1,000 Theta nodes. They also continue to work with ALCF Data Science Program projects to leverage Balsam for machine learning and workflow needs on Mira, Theta, and future systems.

IMPACT Balsam provides a service that simplifies the task of running large-scale job campaigns on supercomputers for production science, allowing users to shift their attention from managing job submissions to focusing on their science. In addition, Balsam gives the ALCF opportunities to optimize job placement and possibly improve system utilization.

PUBLICATIONS

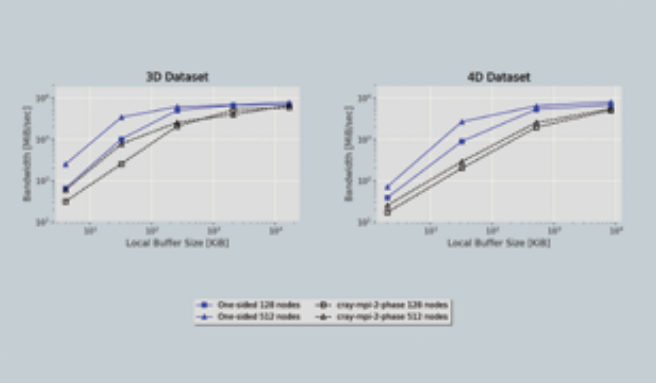
Childers, J.T., T. D. Uram, D. Benjamin, T. J. LeCompte, and M. E. Papka. "An Edge Service for Managing HPC Workflows." *Proceedings of the Fourth International Workshop on HPC User Support Tools - HUST'17* (2017).

Salim, M., T. D. Uram, J. T. Childers, P. Balaprakash, V. Vishwanath, and M. E. Papka, "Balsam: Automated Scheduling and Execution of Dynamic, Data-Intensive HPC Workflows." *PyHPC Workshop, Supercomputing 2018* (submitted).

Computer Science

ExaHDF5: Delivering Efficient Parallel I/O on Exascale Computing Clusters

PI Suren Byna
INST Lawrence Berkley National Laboratory
HOURS ALCC, 1 Million Core-Hours



Performance comparison of the new HDF5 VFD, using one-sided aggregation, with the default binding to Cray MPICH MPI-IO. Data was collected on Theta using an I/O benchmarking tool (the HDF5 Exerciser), developed by ALCF researchers for the ExaHDF5 project. There is a clear performance benefit of one-sided aggregation for many relevant data sizes. *Image: Rick Zamora, Argonne National Laboratory*

As part of DOE's Exascale Computing Project (ECP), researchers are using DOE leadership computing resources to develop exascale-capable applications and to optimize various components of the exascale software stack. For one of ECP's software technology projects, a multi-institution research team is working with Hierarchical Data Format 5 (HDF5), the most popular library for scientific applications to write and read data files, to deliver efficient parallel I/O capabilities on upcoming exascale architectures.

CHALLENGE Parallel I/O, the key technology behind moving data between compute nodes and storage, faces monumental challenges from new application workflows as well as memory, interconnect, and storage architectures considered in the designs of exascale systems. To ensure scientific applications can efficiently access and manage increasingly large datasets, the ExaHDF5 team must overcome challenges in developing I/O strategies for using a hierarchy of storage devices and topology of compute nodes efficiently, developing interoperability features with other file formats, and integrating existing prototyped features into production releases.

APPROACH The ExaHDF5 team, comprising researchers from Argonne National Laboratory, Lawrence Berkeley National Laboratory, and the HDF Group, is using DOE computing resources, including the ALCF's Theta system, to develop new capabilities in HDF5. Their work includes productizing features and techniques that have been previously prototyped, exploring optimization strategies on upcoming architectures, and maintaining and optimizing existing HDF5 features tailored for ECP applications.

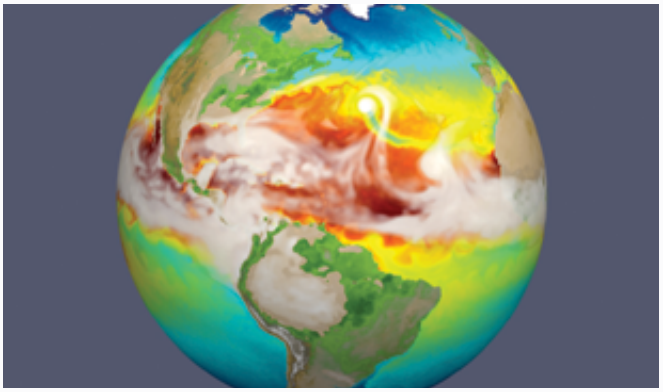
RESULTS Thus far, the team's research has included work on topology-aware data-movement algorithms and collective I/O optimizations within a new HDF5 virtual file driver (VFD). The researchers have also collaborated with Cray developers to merge several performance improvements into Cray's proprietary MPICH MPI-IO. These changes will benefit applications using both MPI-IO and parallel HDF5 on current and future supercomputing systems. In addition, the team has been working with various ECP-funded applications to improve read/write performance.

IMPACT The enhanced HDF5 software will achieve efficient parallel I/O on exascale systems in ways that will impact a large number of DOE science and industry applications. Many of the ECP-funded applications and co-design centers require HDF5 for their I/O, and improving the HDF5 software to handle the unique challenges of exascale architectures will play an instrumental role in the success of the ECP.

Earth Science

Accelerated Climate Modeling for Energy (ACME)

PI Mark Taylor
INST Sandia National Laboratories
HOURS INCITE, 179 Million Core-Hours
(ALCF: 89M; OLCF: 90M)



Hurricane in North-Central Atlantic shown with resultant cold water (green) in warm Central Atlantic (red). *Image: Mark Taylor, Sandia National Laboratories*

With the coming paradigm shift in computer architectures and programming models as capability moves to the exascale era, the Accelerated Climate Modeling for Energy (ACME) project (now known as the Energy Exascale Earth System Model, or E3SM) aims to develop a cutting-edge climate and earth system that can tackle the most demanding climate research imperatives. By harnessing the supercomputing resources of the ALCF, a group of researchers led by Sandia National Laboratories is addressing questions concerning the water cycle and cryosphere systems.

CHALLENGE The research team first seeks to simulate changes in the hydrological cycle, specifically focusing on precipitation and surface water in regions where this cycle is impacted by complex topography (such as the western United States and the headwaters of the Amazon). The second objective is to determine the possibility of dynamical instability in the Antarctic Ice Sheet appearing sometime in the next 40 years.

APPROACH The team made extensive use of Theta to run the recently released E3SM code, which comprises component models for atmosphere, ocean, sea ice, and land. Sixty-four tasks were assigned to every node, each with two OpenMP threads so as to establish intranodal parallelism.

The majority of the cores were allocated to the atmosphere model, a subset of which also ran the land and sea models; the remaining cores were allocated to the ocean model, which runs concurrently with the atmosphere model. Its examination of the risk of Antarctic Ice Sheet collapse represents the first fully coupled simulation to include dynamic ocean-ice shelf interactions.

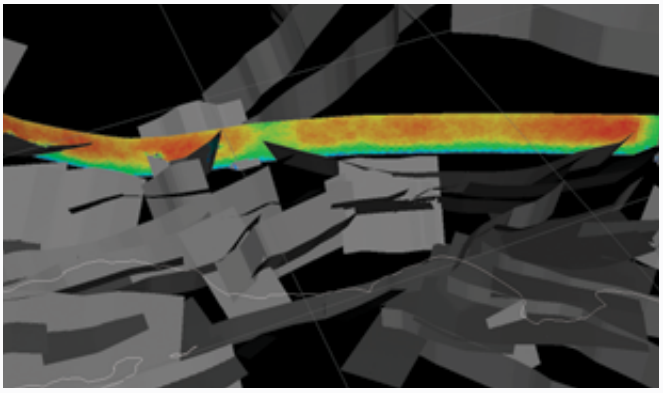
RESULTS The researchers conducted several simulations ranging from three to five years in length so as to test different atmospheric tunings and initial conditions for ocean and ice. Beyond allowing evaluation of the model, this testing also allowed for workflow development and prepared the team for deeper studies.

IMPACT In addition to further advancing the predictive power of climate models and providing insight into the climatic effects of rapid changes in the earth's ice content, the E3SM simulations have the potential to answer how water resources and the hydrological cycle interact with the climate system on both local and global scales. Hurricane hindcast simulations performed for this project demonstrated the high fidelity with which extreme weather can be modeled, while exposing parametric weaknesses that need improvement.

Earth Science

Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations

PI Thomas H. Jordan, Christine Goulet
INST University of Southern California
HOURS INCITE, 126 Million Core-Hours
(*ALCF: 30M; OLCF: 96M)*



3D view of a magnitude 7.9 earthquake on the Southern San Andreas Fault from an RSQSim simulation. Colors indicate elements that slipped in the earthquake, brighter colors indicating areas of higher slip. Faults that did not participate in this event are shown in gray. *Kevin Milner, University of Southern California*

Having accurate seismic hazard information is vital in order to maintain human and economic safety in seismically active regions. This INCITE project uses DOE computing resources to develop more accurate physics-based simulations of earthquake rupture and wave propagation to forecast ground motions at frequencies of interest to civil engineers. This allows improved understanding of earthquake processes and helps reduce uncertainties compared to existing seismic hazard estimates.

CHALLENGE Human and economic risks in seismically active regions continue to increase as urban areas and their dependence on interconnected infrastructure networks continues to grow. Understanding seismic hazards across a wide spectrum of forecasting and response times, including a proper assessment of modeling uncertainties, is the foundation on which most seismic risk-reduction strategies are developed. Improved geological models and extension of new techniques to higher frequencies allow greater fidelity hazard estimation, but they also require extensive use of high performance computing.

APPROACH In this INCITE project, the team is using Mira to run the earthquake simulator code RSQSim, which produces long synthetic earthquake catalogs, on the order of millions of years. A baseline simulator model was developed with globally uniform model parameters tuned to match observed earthquake scaling.

RESULTS Using RSQSim, the team further developed and refined earthquake simulator models of the California fault system, comparing results from the simulator against state-of-the-art UCERF3 (Uniform California Earthquake Rupture Forecast 3). As an initial comparison, a series of hazard-relevant measures were made, combining both earthquake rupture forecasts with ground motion prediction equations. While at first the intent was to evaluate the magnitude of differences between the models, the SCEC team instead found very good agreement. Averaged over a representative set of sites, the RSQSim-UCERF3 hazard-curve differences are comparable to the small differences between UCERF3 and its predecessor, UCERF2. This agreement provides a fundamental verification at the system level for both approaches and is anticipated to markedly improve seismic hazard estimates and their uncertainties.

IMPACT This research is leading to more accurate physics-based simulations of earthquake rupture and wave propagation, and improved analyses, by adding new elements and enhancing existing features in the models. Results are expected to improve seismic hazard information products that have broad impact, including seismic hazard maps and civil engineering design codes.

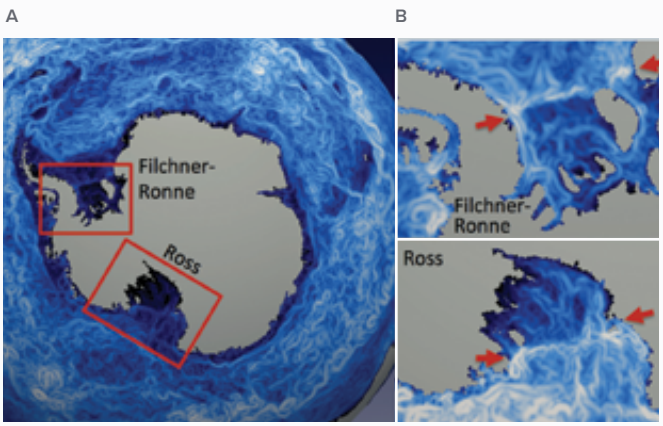
PUBLICATIONS

Shaw, B. E., K. R. Milner, E. H. Field, K. Richards-Dinger, J. J. Gilchrist, J. H. Dieterich, and T. H. Jordan. "A Physics-Based Earthquake Simulator Replicates Seismic Hazard Statistics Across California," *Science Advances* (August 2018), AAAS.

Earth Science

Understanding the Role of Ice Shelf-Ocean Interactions in a Changing Global Climate

PI Mark Petersen
INST Los Alamos National Laboratory
HOURS ALCC, 87 Million Core-Hours
(ALCF: 25M; OLCF: 2M; NERSC: 60M)



Ocean speed from E3SM simulation shows significant eddy activity throughout the Southern Ocean. Right panels reveal currents near and below the Filchner-Ronne and Ross ice shelves. The shelf edge is denoted by arrows. White currents indicate column-integrated speeds of **(A)** 500-2000 m^2/s and **(B)** 30-100 m^2/s. *Image: Mark Petersen, Los Alamos National Laboratory*

Evaluating the likelihood of rapid sea-level rise due to mass loss from the Antarctic Ice Sheet (AIS) is one of the primary motivations for the DOE's Energy Exascale Earth System Model (E3SM) project. Evidence suggests that the AIS is particularly vulnerable to effects that result from the reduced buttressing (suppression of ice flow) of warming ice shelves. In light of this, researchers from Los Alamos National Laboratory are introducing new models that simulate the key processes in global ocean circulation responsible for delivering warm waters to the AIS base.

CHALLENGE Simulating AIS-related sea-level change requires deepened understanding of both the global climate's influence on ocean-induced melting under ice shelves and feedbacks between ice-shelf meltwater, ocean circulation, and the global climate. With this in mind, the team's simulations are intended to (a) validate the E3SM model in a configuration incorporating ocean cavities under ice shelves; (b) demonstrate the influence of the global climate on sub-ice shelf melting; (c) investigate the relevance of ice shelf-ocean processes to the global climate; and (d) explore the likely effect of climate change on sub-ice shelf melt rates (and, inferentially, ice-sheet stability). Ice-shelf cavities have not been included in prior fully coupled global climate models, largely because of computational and coupling challenges, thereby highlighting the necessity of ALCF leadership-class resources.

APPROACH The researchers are using Theta to run E3SM, which is created for variable-resolution meshes and includes ocean, sea-ice, land ice and atmospheric components. E3SM is designed to run efficiently on HPC platforms using MPI, OpenMP, Fortran and C, and scales well to 10,000–50,000 processors.

RESULTS The team has demonstrated that global earth system simulations with high spatial resolution and ice shelf cavities lead to improved representation of ocean properties proximal to and beneath the ice shelves. This results in ice shelf melt rates that are closer to observed values.

IMPACT Sea-level rise will be one of the costliest impacts of climate change, as coastal regions serve half of the nation's population and contain vital infrastructure vulnerable to increased flooding. Improved understanding of physical processes below Antarctic ice shelves leads to more accurate projections of melt rates and ocean circulation, and these are important components of sea level rise.

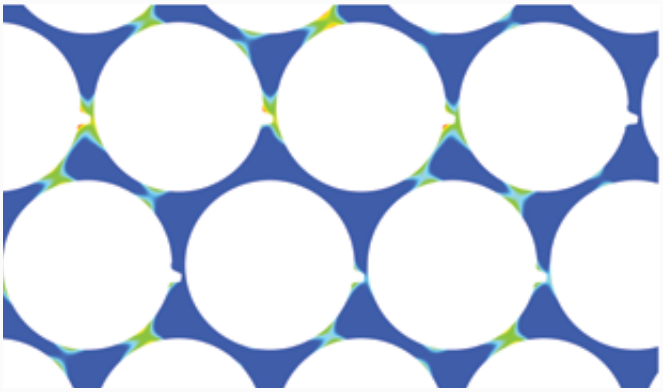
PUBLICATIONS

Petersen, M., X. Asay-Davis, A. Berres, Q. Chen, N. Feige, D. Jacobsen, P. Jones, M. Maltrud, T. Ringler, G. Streletz, A. Turner, L. Van Roekel, M. Veneziani, J. Wolfe, P. Wolfram, and J. Woodring. "An Evaluation of the Ocean and Sea Ice Climate of E3SM Using MPAS and Interannual CORE-II Forcing," *Journal of Advances in Modeling Earth Systems* (May 2018), Wiley.

Energy Technologies

High-Fidelity Multiphysics Simulations to Improve Nuclear Reactor Safety and Economics

PI Emily Shemon
INST Argonne National Laboratory
HOURS ALCC, 44 Million Core-Hours



Temperature distribution in 91-pin wire-wrapped fuel bundle from the AFR-100 sodium-cooled fast reactor design, calculated by PROTEUS/Nek5000. Hot spots are observed where the wire-wrap contacts the fuel cladding due to decreased coolant velocity in that vicinity. *Image: Yiqi Yu, Argonne National Laboratory*

With the ability to recycle used nuclear fuels, fast reactors are a promising nuclear energy technology that can substantially reduce radioactive waste and efficiently utilize natural nuclear resources. It is a top priority of the DOE to accelerate the design of safe and economical fast reactors, which offer great potential as a sustainable, domestic energy source. In this ALCC project, the team is using ALCF computing resources to accurately assess the safety parameters of fast reactor designs through high-fidelity multiphysics modeling.

CHALLENGE This project aims to eliminate various modeling and simulation uncertainties in the calculation of a safety parameter called hot channel factors, which have historically been assessed using low-fidelity legacy physics solvers coupled with expensive mockup experiments. Today's high-fidelity multiphysics tools offer improved accuracy over conventional techniques without the aid of expensive experiments, but they require the use of high-performance computing systems.

APPROACH The researchers are using the DOE-NEAMS (Nuclear Energy Advanced Modeling and Simulation) developed SHARP Toolkit, which includes the PROTEUS neutronics code and the Nek5000 thermal hydraulics/computational fluid dynamics code, to carry out their high-fidelity multiphysics calculations. To reduce computational cost, this project also assessed a "zooming" tool for core simulations called SHARP Zoom, where local regions of interest are represented with full fidelity and other regions are represented with much coarser geometry. The use of ALCF supercomputers for these simulations allows for more accurate geometry and physics representations of the system than achieved with the legacy solvers.

RESULTS The team has successfully reduced or eliminated numerous modeling and simulation uncertainties, resulting in reduced hot channel factors compared to conservative legacy estimates. Smaller hot channel factors enlarge the safety margin to design limits or permit the reactor to operate at higher power, hence increasing economic output. The team also showed that SHARP Zoom has the potential to zoom anywhere in the core, making detailed information available at a fraction of the cost of a fully heterogeneous multiphysics core calculation and thereby greatly expanding the usability of high-fidelity tools in the field.

IMPACT This project demonstrates high-fidelity modeling capabilities that can improve the economics and safety of advanced fast reactor designs, which supports DOE's mission to facilitate the commercial deployment of such reactors as a clean and sustainable energy source.

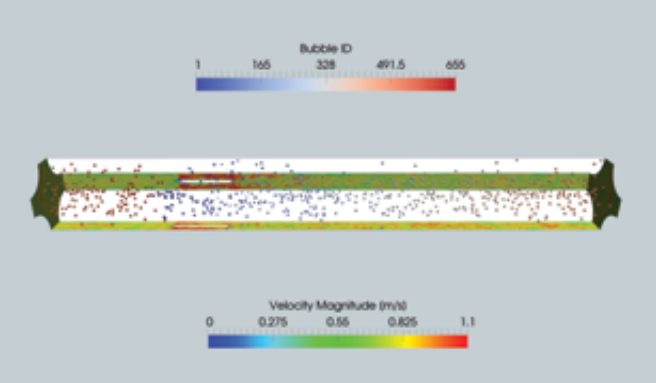
PUBLICATIONS

Shemon, E. R., Y. Yu, T. K. Kim, and A. J. Mausolff. "High Fidelity Multiphysics Calculations of Hot Channel Factors for Sodium-Cooled Fast Reactors", *Proceedings of PHYSOR 2018: Reactor Physics Paving the Way Towards More Efficient Systems* (April 2018).

Energy Technologies

Multiphase Simulations of Nuclear Reactor Flows

PI Igor Bolotnov
INST North Carolina State University
HOURS ALCC, 130 Million Core-Hours



Turbulent two-phase flow simulation of 655 resolved bubbles within a PWR subchannel. *Image: Jun Fang, Argonne National Laboratory*

Boiling phenomena, bubble formation, and two-phase (liquid/gas) flow in nuclear reactor geometries are important physical processes that affect nuclear reactor safety. In particular, high bubble concentrations in pressurized water reactor (PWR) designs can lead to a phenomenon called departure from nucleate boiling and cause overheating and disintegration of the fuel if the fluid conditions are not designed properly. A team led by North Carolina State University researchers will use direct numerical simulations of fully resolved deformable bubbles at unprecedented scale (powered by ALCF leadership-class computers) to study boiling and flow processes in nuclear reactor geometries and answer fundamental questions about the interface of flow phases and turbulence.

CHALLENGE The project has two objectives: (1) perform smaller simulations to obtain statistically steady state conditions and extract physically-based numerical data for the development of coarser scale models; and (2) perform cutting-edge, large-scale runs to demonstrate the newly developed advanced methodologies of in-situ bubbly flow data collection and post-processing.

APPROACH Fully resolved bubbly flow fields in PWR fuel assembly sub-channels with spacer grids and mixing vanes were performed on meshes exceeding one billion elements to approach the operating conditions in nuclear reactor cores in terms of Reynolds numbers and bubble sizes. To achieve this level of fidelity, the massively parallel finite element-based flow solver PHASTA incorporates the level-set method to resolve bubbly flows in nuclear core geometries.

RESULTS Results from the first objective were extensively used by DOE's Consortium for Advanced Simulation of Light Water Reactors (CASL) program to develop a new generation of boiling models to be included in CASL's virtual reactor multiphysics model. Additionally, the simulations produced detailed distributions of bubble concentration and estimated the variation of the forces acting on the bubbles, providing novel insight into understanding two-phase flow. The large-scale runs from the second objective successfully demonstrated the new bubble tracking approach, as well as the data processing and collecting techniques at scale for future simulations.

IMPACT The improved boiling phenomena models directly contribute to CASL's mission of developing advanced modeling and simulation tools to improve the operation and safety of the existing nuclear fleet. These efforts are transitioning the historically conservative nuclear industry to adopt novel approaches in reactor analysis, which are crucial for successful next-generation reactor designs.

PUBLICATIONS

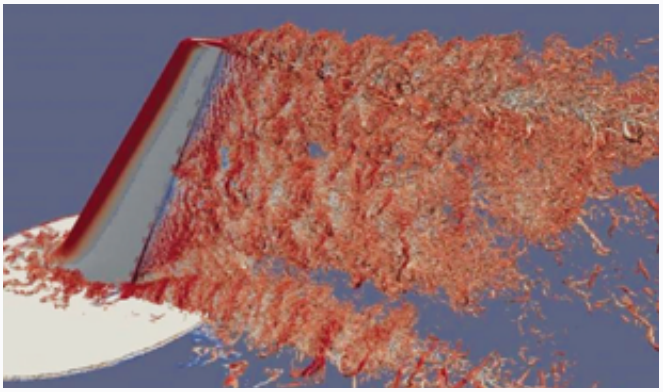
Fang, J., J. J. Cambareri, C. S. Brown, J. Feng, A. Gouws, M. Li, and I. A. Bolotnov. "Direct Numerical Simulation of Reactor Two-Phase Flows Enabled by High-Performance Computing," *Nuclear Engineering and Design* (April 2018), Elsevier.

Fang, J. and I. A. Bolotnov. "Bubble Tracking Analysis of PWR Two-Phase Flow Simulations Based on the Level Set Method," *Nuclear Engineering and Design* (November 2017), Elsevier.

Engineering

Adaptive DDES of a Vertical Tail/Rudder Assembly with Active Flow Control

PI Kenneth Jansen
INST University of Colorado Boulder
HOURS INCITE, 208 Million Core-Hours
(ALCF: 200M; OLCF: 8M)



Instantaneous isosurface of vorticity (Q) from a detached eddy simulation of a vertical tail/rudder assembly with flow control from a single, active synthetic jet (5th from root). Five billion elements resolve the flow control interaction with the separated flow on the rudder using 128 Ki processors. *Image: Kenneth Jansen, University of Colorado Boulder*

Throughout history, understanding fluid flow has proved to be one of the greatest challenges in all of science. With the power of the ALCF's supercomputers at their disposal, a team of researchers led by the University of Colorado Boulder are advancing computational modeling capabilities to provide deeper insight into the opaque problems posed by fluid flow and how their resolution can lead to refined aircraft design.

CHALLENGE Viscous effects near aerodynamic bodies (such as airplanes) create highly anisotropic (that is, directionally dependent) solutions to the partial differential equations governing fluid flow. This motivates the use of higher-order discretization methods, which minimize numerical dissipation and dispersion errors, to allow for more accurate modeling of the flow turbulence. However, the added complexity makes scalable implementation on parallel processors more difficult—the successful realization of which leads to higher fidelity solutions than those obtained from the more commonly used lower-order discretization methods (e.g. unstructured mesh, second-order finite volume codes).

APPROACH Using Theta and Mira, the research team collaborated with ALCF staff to improve the performance of the computational fluid dynamics analysis package PHASTA. PHASTA was paired with discretizing approximation methods known as adaptive meshing procedures to refine regions of the flow with high turbulence anisotropy.

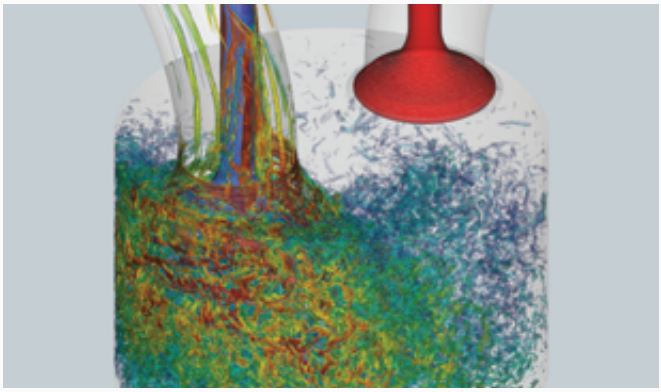
RESULTS Comparisons with experimental data corroborated the accuracy of the simulations and the efficiency of the code, validating the team's efforts to achieve code scalability. The results indicate that the team is on the right path to perform flight-scale simulations on Aurora once that system is available. The researchers are currently working on simulations featuring more complex turbulence conditions (corresponding to a Reynolds number of 700,000).

IMPACT By helping to realize the goals of aerodynamic design (which is to say, improving aircraft performance) with the introduction of a powerful predictive tool, this project can reduce the size and weight of aircraft tails and rudders, as well as their drag contributions during cruise conditions. This would result in a potentially massive reduction in fuel use, thereby lowering both emissions and expenditures.

Engineering

Low-Mach Simulation of Flow and Heat Transfer in an Internal Combustion Engine

PI Saumil Patel
INST Argonne National Laboratory
HOURS DD, 7 Million Core-Hours



Visualization of vortical flow structures during the intake stroke of an internal combustion engine. *Image: George Giannakopoulos, ETH-Zürich*

The enhanced understanding of the turbulent flow, heat transfer, and combustion in internal combustion engines will enable the development of advanced designs with higher efficiency and reduced greenhouse gases and pollutant emissions. A team of researchers from ETH-Zürich, Argonne National Laboratory, the University of Illinois at Urbana-Champaign, and the Aristotle University of Thessaloniki in Greece is using ALCF supercomputers to develop a scalable high-fidelity simulation methodology to shed light on the complex processes taking place inside internal combustion engines.

CHALLENGE The investigation of the interaction of multiple physical phenomena (turbulence, heat transfer, compressibility) interacting across a large range of time and length scales in a domain with moving boundaries (pistons, valves) is computationally very intensive, and necessitates the use of high-performance computing systems.

APPROACH The research team is using Mira and Theta to extend the capabilities of Nek5000, a high-order, scalable computational fluid dynamics solver developed at Argonne, to simulate turbulent flow and thermal fields inside realistic engine geometries. Numerical algorithms were developed and implemented to accurately account for the complex piston and valve motion, and to reduce the time-to-solution for the simulation of multiple engine cycles.

RESULTS The simulation campaign captured the in-cylinder flow and heat transfer within the Transparent Combustion Chamber (TCC)-III experimental engine designed by General Motors. Running the enhanced Nek5000 code on ALCF supercomputers allowed the team to simulate fluid length-scales as small as .03 mm in about 12 hours per engine cycle. The simulation of 34 cycles of the gas exchange process revealed variations in the intake jet penetration and angle from cycle to cycle, and allowed for the characterization and quantification of the in-cylinder, large-scale motion and break down during compression. The calculations confirm increasing levels of turbulence, which is crucial to efficient engine operation. The team was recently awarded an ALCC allocation to continue to advance the use of Nek5000 for engine simulations.

IMPACT The project demonstrates a highly accurate and scalable approach for simulating the complex phenomena occurring inside internal combustion engines. By providing precise predictions with a short turnaround time, this method can help to advance the design of more efficient engines.

PUBLICATIONS

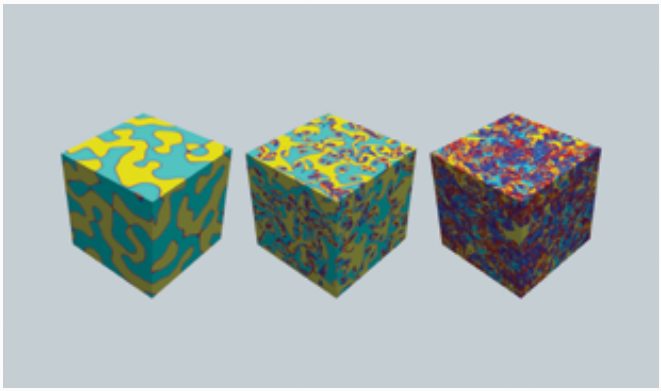
Giannakopoulos, G. K., C. E. Frouzakis, S. Patel, P. F. Fischer, A. G. Tomboulides, and K. Boulouchos. "LES of the Gas-Exchange Process Inside an Internal Combustion Engine Using a High-Order Method," *12th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements* (2018).

Giannakopoulos, G. K., S. Patel, C. E. Frouzakis, P. F. Fischer, A. G. Tomboulides, and K. Boulouchos. "Study of the Cyclic Flow Variability in an IC Engine Using Spectral Elements," *Platform for Advanced Scientific Computing Conference* (2018).

Engineering

Non-Boussinesq Effects on Buoyancy-Driven Variable-Density Homogeneous Turbulence

PI Daniel Livescu
INST Los Alamos National Laboratory
HOURS ALCC, 60 Million Core-Hours



3D visualization of the evolution of the mole fraction for the density ratio 1.105:1 with 2048^3 simulation, as two initially segregated fluids mix and generate turbulence. *Image: Denis Aslangil and Arindam Banerjee, Lehigh University; Daniel Livescu, Los Alamos National Laboratory*

Fluids with different densities blend together to create a homogeneous mixture in a multitude of important applications, from atmospheric and oceanic flows to combustion and supernova formation. Despite its universal occurrence, the resulting turbulence remains a largely unstudied phenomenon. Researchers from Los Alamos National Laboratory and Lehigh University are breaking ground in fluid dynamics by using ALCF supercomputers to shed light on this little-understood process.

CHALLENGE Due to its relative ubiquity, the mixing of two or more miscible fluids with different densities is of fundamental interest and represents a canonical flow problem. The researchers sought to investigate, via high-resolution direct numerical simulations (DNS) on ALCF supercomputers, the effects a high density-ratio has on buoyancy-driven homogeneous variable-density turbulence (HVDT). Density discrepancies among materials result in a mixing scenario distinct from when materials share the same density.

APPROACH The team used Mira to run a variable-density version of the primarily Fortran-based code CFDNS. This version of the code solves continuity and compressible momentum transport equations coupled to a divergence condition for the velocity field due to the variable-density mixing. This condition results in a Poisson equation with variable coefficients, for which the team devised efficient solvers where Fast Fourier Transforms are used to evaluate spatial derivatives.

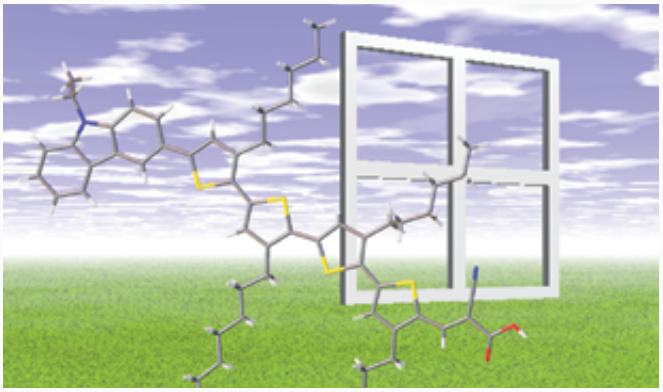
RESULTS The researchers ran DNS with higher Atwood numbers and resolutions than had previously been performed. Larger density ratios were found to cause different mix rates within the different flow regions and to change the turbulence structure. Energy conversion efficiency was discovered to be highly dependent on the density ratios of mixing fluids: lower Atwood numbers more efficiently generate turbulent kinetic energy during explosive growth (early time turbulence growth), but the energy conversion efficiencies peak at Atwood values between 0.25 and 0.5 during saturated growth (later time of the turbulence growth). Buoyance-assisted HVDT decay is also found to be significantly different from the classical single-fluid turbulence decay as it occurs at a constant Reynolds number, offering the potential to improve turbulence theory.

IMPACT This research advances basic science. As the examined scenarios are so common, the results stand to impact atmospheric and oceanic sciences, astrophysics, and engineering. These simulations will enable studies of the same phenomena that are seen in practical applications. The researchers will use the generated data to improve variable-density turbulence theory and calibrate turbulence models, and examine strategies for new non-DNS codes.

Materials Science

Data-Driven Molecular Engineering of Solar-Powered Windows

PI Jacqueline Cole
INST University of Cambridge
HOURS ADSP, 117 Million Core-Hours



Abstract representation of solar-powered windows (including molecule designed for dye-sensitized solar cells). *Image: Jacqueline Cole, University of Cambridge*

Building use accounts for some 40 percent of the total energy consumption in the U.S., so embedding new environmental technologies in the cities of the future is paramount to energy sustainability. Smart windows—proposed windows that would generate electricity from sunlight—represent a decisive step in that direction. To make smart windows a reality, University of Cambridge researchers are exploiting large-scale data mining with machine learning to discover more effective light-absorbing molecules that can be used to construct dye-sensitized solar cells.

CHALLENGE This project's central component lies in data source generation, which intelligently pairs together a concerted set of experimental and computational data on the structures and optical properties of 80,000 molecules, mined by a database auto-generation tool, ChemDataExtractor, that the researchers have developed. The computational data on these molecules complements the experimental data by providing optical properties and quantum energy information; obtaining such data requires the use of the ALCF's Theta machine in order to run high-throughput density functional theory (DFT) and time-dependent DFT calculations. Once these calculations are complete, the obtained data can be mined with algorithms that target materials with optimal function, yielding a shortlist of dye candidates ready for experimental validation.

APPROACH An initial set of data was extracted using ChemDataExtractor. Dye pairs conducive to complementary optical absorption (pairs that yield overall panchromatic light absorption) were then algorithmically matched. NWChem calculations were performed on Theta to aid the final stage of data-mining, enabling materials prediction of optimal dyes for co-sensitization. This process narrowed the initial list of more than 9,000 dye candidates down to a mere six.

RESULTS Chemistry groups from around the world synthesized the six dyes predicted to have solar-cell prospects; co-sensitization experiments and materials characterization are underway to optimize them for solar-cell device fabrication and testing.

Additionally, the researchers have detailed in *ACS Applied Materials and Interfaces* their discovery of a chemical bond in a related dye, to which that dye's attractive photovoltaic properties can be attributed.

IMPACT Buildings are the centerpiece of modern living. As demand for energy continues to increase, solar-powered smart windows have emerged as a promising technology to power our cities in a sustainable, environmentally friendly fashion. By discovering ideal materials for the windows' manufacture, this project helps innovate this technology.

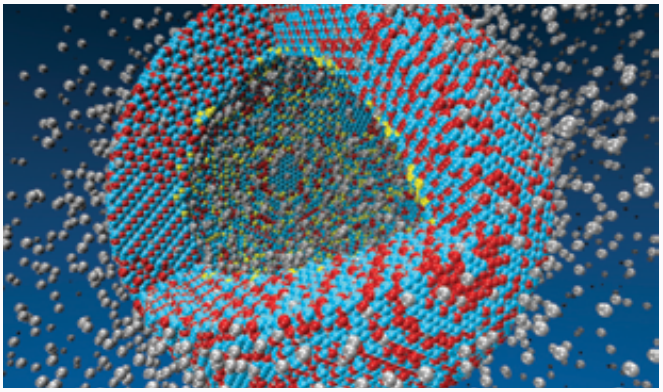
PUBLICATIONS

Cole, J. M., M. A. Blood-Forsythe, T.-C. Lin, P. Pattison, Y. Gong, Á. Vázquez-Mayagoitia, P. G. Waddell, L. Zhang, N. Koumura, and S. Mori. "Discovery of S···C=N Intramolecular Bonding in a Thiophenylcyanoacrylate-Based Dye: Realizing Charge Transfer Pathways and Dye···TiO_2 Anchoring Characteristics for Dye-Sensitized Solar Cells," *ACS Applied Materials and Interfaces* (July 2017), American Chemical Society.

Materials Science

Imaging Transient Structures in Heterogeneous Nanoclusters in Intense X-Ray Clusters

PI Phay Ho
INST Argonne National Laboratory
HOURS ALCC, 68 Million Core-Hours



The snapshot of ionization dynamics of iron oxide nanoparticle with Mo distributed randomly in the inner layer at the peak of the laser pulse, where the red, cyan, yellow and silver particles are O, Fe, Mo and electron respectively. The 8.6-keV XFEL pulse has a pulse fluence of 10^{13} photons/μm^2 and pulse duration of 10 fs. *Image: Phay Ho, Argonne National Laboratory*

High-brightness X-ray free-electron laser (XFEL) pulses provide researchers with unprecedented tools to observe the dynamics of atoms and electrons with atomic spatial resolution. Researchers from Argonne National Laboratory aim to develop a quantitative and predictive understanding of X-ray matter interactions in nanosized heterogeneous systems on an atomistic level: Characterizing the complex phenomena that emerge can subsequently guide future experimental strategies.

CHALLENGE The main objective is to examine, with high-intensity X-ray laser pulses, the correlation between sample excitation and the degree of achievable inner contrast and spatial resolution. By exploiting sample heterogeneity with these pulses, the researchers hope to control the ultrafast transient electronic and nuclear dynamics that occur.

APPROACH To address the challenges associated with tracking particle motion and the evolution of electronic configurations, the team has employed a hybrid Monte Carlo/Molecular Dynamics (MC/MD) algorithm. With this highly parallelized code (written in C/C++ with MPI and OpenMP), the coordinates and velocities of all particles are propagated via MD, while the electronic transitions are sampled according to MC. This method has been implemented in LAMMPS. Each step in the simulation updates all particle coordinates as a function of forces derived from interaction potentials. At each MC step, however, an MC procedure incorporates quantum effects via cross-sections and evaluates probabilities for photoionization, resonant excitation, inner-shell relaxation collisional ionization, and electron-ion recombination. A new parallelization strategy for this method is underway.

RESULTS The researchers performed MC/MD calculations to compute the scattering response of core-shell iron oxide nanoparticles doped with molybdenum atoms in four different distributions, with the goal of investigating the feasibility of imaging the distribution of dopants within the nanoparticles using an XFEL single-particle technique. The calculations included the effects of ionization and the overall sample excitation of electron and nuclear dynamics, enabling the determination of the ideal pulse condition for the single-particle imaging experiment.

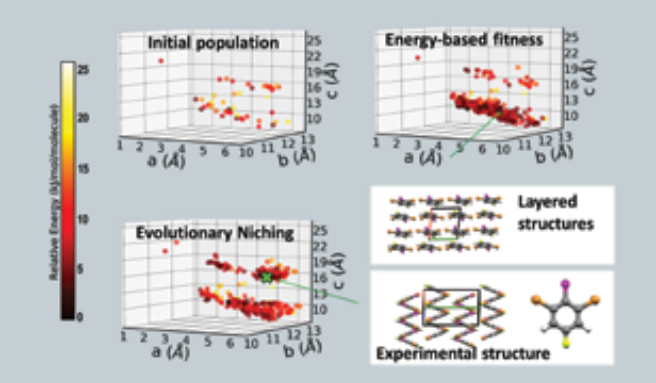
The obtained results have led to a proposal to perform a single-particle imaging experiment at the European XFEL facility to image the structure and dopant distribution of core-shell iron oxide nanoparticles with both atomic and elemental resolution.

IMPACT This research will permit significant expansion of our understanding of the non-linear X-ray regime (interactions on the X-ray wavelength remain largely unexplored in physics) and guide the experimental efforts and future capabilities of XFEL facilities.

Materials Science

Materials and Interfaces for Organic and Hybrid Photovoltaics

PI Noa Marom
INST Carnegie Mellon University
HOURS INCITE, 261 Million Core-Hours
(ALCF: 230M: OLCF: 31M)



Evolutionary niching helps GAtor find the experimental structure of 1,3-dibromo-2-chloro-5-fluorobenzene. Reproduced from Faraday Discussions, DOI: 10.1039/C8FD00067K (2018). *Image: Farren Curtis, Noa Marom, and Timothy Rose, Carnegie Mellon University*

Organic and hybrid organic-inorganic photovoltaics are a promising alternative to silicon solar cells for certain applications. The discovery and design of such materials pose steep demands, making predictive computer simulations an ideal tool for development. An international research team from Carnegie Mellon University, Duke University, Aalto University, Technical University Graz, and Technical University Munich are leveraging ALCF supercomputers to revolutionize not only solar energy, but materials discovery at large via new computational paradigms.

CHALLENGE Because structure determines function, the design of functional materials needs to occur on the atomic level, yielding possible structural combinations too numerous for experimental fabrication. The most viable option for discovery is recourse to simulations based on first-principle quantum-mechanical approaches. Such simulations require massively parallel high-performance computers, offered by the ALCF.

APPROACH To guide material discovery, the INCITE research team is pairing the density-functional code FHI-aims, which determines electronic structure, with a set of optimization algorithms that predict materials structure, including the genetic algorithm (GA) GAtor. GAs operate by mimicking the evolutionary process. The target property is mapped onto a fitness function. Structures with a high fitness have an increased probability to "mate," whereby a crossover operator combines the structural "genes" of the parent structures to produce a child structure, which is then added to the population. The process repeats iteratively until an optimum is found. The calculations are running on Mira and Theta.

RESULTS As detailed in a paper published in *Faraday Discussions*, the researchers implemented evolutionary niching in GAtor to enable multimodal optimization. Machine learning algorithms are used to dynamically cluster the population by structural similarity. A cluster-based fitness function is then used to steer the GA towards promising under-sampled regions of the configuration space. This reduces initial population and selection biases and improves the GA performance.

IMPACT What this project accomplishes could create breakthroughs in the ways we generate solar energy, while also broadly advancing materials and data sciences. It will lead to a deeper fundamental understanding of atomic-level structural property relations, in addition to preparing versatile, parallelized codes ready for the next generation of supercomputers. Moreover, the datasets produced will be made publicly available, thereby establishing a bedrock for further simulation-based materials discovery.

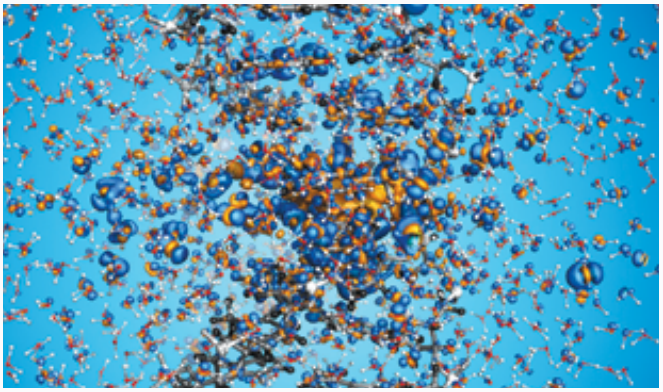
PUBLICATIONS

Curtis, F., T. Rose, and N. Marom. "Evolutionary Niching in the GAtor Genetic Algorithm for Molecular Crystal Structure Prediction," *Faraday Discussions* (April 2018), Royal Society of Chemistry.

Materials Science

Modeling Electronic Stopping in Condensed Matter Under Ion Irradiation

PI Yosuke Kanai
INST University of North Carolina at Chapel Hill
HOURS INCITE, 155 Million Core-Hours
(ALCF: 140M; OLCF: 15M)



A snapshot from non-equilibrium electron dynamics simulation of DNA in water under proton irradiation. The blue and orange isosurface represents areas with positive and negative changes in electron density with respect to the equilibrium density. *Image: Dillon C. Yost, University of North Carolina at Chapel Hill*

Electronic stopping refers to the dynamical transfer of kinetic energy from energetic charged particles (e.g. protons) to electrons in a target material, consequently inducing massive electronic excitations therein. Elucidation of this phenomenon as it occurs in condensed matter systems under ion irradiation contributes to impactful breakthroughs in a number of modern technologies. A team of researchers from University of North Carolina at Chapel Hill, University of Illinois at Urbana-Champaign, and Lawrence Livermore National Laboratory are using predictive simulations to model electronic stopping dynamics in semiconductors due to their importance in various applications such as proton-beam cancer therapy.

CHALLENGE Predictive modeling of electronic stopping processes has remained a great challenge for many decades because of the difficulties involved in accurately describing the excitation of electrons; however, recent innovations in first-principles quantum-mechanical methodologies and massively parallel supercomputers have enabled precise simulations of these processes. The researchers now seek to further advance simulation capabilities so as to model complex systems like semiconductors and solvated DNA under various ion irradiations. A new challenge is to elucidate and correctly describe the role played by the (semi-)core electrons of projectile ions in cases of heavy ion radiations.

APPROACH This project continues to develop a highly scalable implementation of real-time, time-dependent density functional theory using the Qbox/Qb@ll code. Hundreds of thousands of processors in the Mira and Theta systems are used to simulate the quantum-mechanical electronic response of complex systems (for instance, solvated DNA with over 13,000 electrons under ion irradiation).

RESULTS Studying magnesium oxide under silicon ion irradiation, the researchers examined the important role of core-electron excitation and transfer. The team also made significant progress highlighting the differences between the electronic response of DNA irradiated with protons and alpha-particles. The simulations have shown, for example, that holes generated in DNA are strongly localized along the projectile ion path, which primarily excites valence electrons, in contrast to when they are exposed to photon-based ionizing radiations like X-rays and gamma-rays, which excite semi-core and core electrons, respectively.

IMPACT Greater understanding of electronic stopping processes at the microscopic scale will advance a variety of modern technologies, including focused-ion beam fabrication, proton-beam cancer therapy, nuclear reactor material design, and the manufacture of advanced electronics such as quantum bits.

Materials Science

Petascale Simulations for Layered Materials Genome

PI Aiichiro Nakano
INST University of Southern California
HOURS INCITE, 200 Million Core-Hours

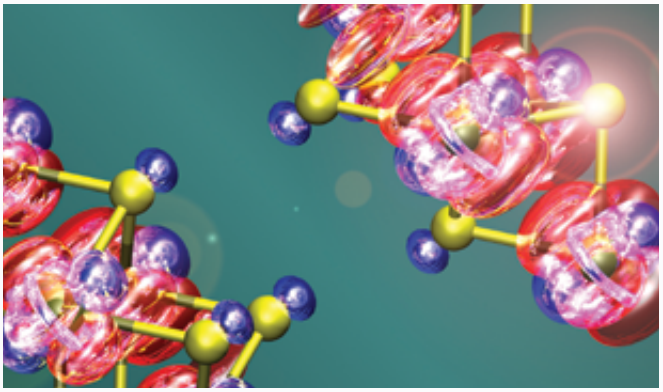


Photo-generated electron (red) and hole (blue) wave functions in bilayer molybdenum diselenide, where gold and yellow spheres are molybdenum and selenium atoms. *Image: Lindsay Bassman, Aravind Krishnamoorthy, and Ken-ichi Nomura, University of Southern California*

By combining highly desirable electronic, optical, magnetic, and chemical properties with an unprecedented degree of specification, functional layered materials will dominate nanomaterials science this century: stacking different material layers, each of which is equipped with optimal properties, enables scientists to fine-tune and exploit their holistic functionality. The crucial role they will play has inspired the Materials Genome Initiative, a multi-agency bid to create a new era of policy, resources, and infrastructure that support the efforts of U.S. institutions to discover, manufacture, and deploy advanced materials faster but at a reduced cost. A team of researchers from the University of Southern California seeks to advance this initiative by using supercomputer-powered simulations to aid in the synthesis of layered materials and elucidate new property relationships.

CHALLENGE This project aims to advance the synthesis of stacked layered materials by chemical vapor deposition, exfoliation, and intercalation; and to discover function-property-structure relationships in the materials, with a special focus on far-from-equilibrium electronic processes.

APPROACH Made possible by ALCF resources, the research team is carrying out nonadiabatic quantum molecular dynamics (NAQMD) and reactive molecular dynamics (RMD) simulations. The simulations are being validated by experiments at SLAC National Accelerator Laboratory's Linac Coherent Light Source (LCLS) and Ultrafast Electron Diffraction (UED) facilities, providing predictive theory to support the DOE-funded MAterials Genome Innovation for Computational Software (MAGICS) center at the University of Southern California. The simulation results will be integrated with MAGICS' computational linguistics and big data analytics efforts to advance efforts to build a layered materials genome.

RESULTS The results of NAQMD simulations corroborating UED experiments were published in *Nature Communications*, while a paper in *Nano Letters* elucidated the mechanism of phonon-mode softening that occurs upon photoexcitation. The researchers are currently investigating the photoexcitation dynamics of 2D materials featuring a substrate.

IMPACT This project advances the DOE's layered materials genome efforts. The simulations, integrated with computational linguistics and big data analytic efforts, will aid in future syntheses of stacked layered materials for a wide range of energy, optoelectronic, and sensor applications, which may lead to entirely novel device fabrication and architecture. Moreover, the discovery of function-property-structure relationships—to be made widely available to other materials scientists—will fuel further advancements and innovation.

PUBLICATIONS

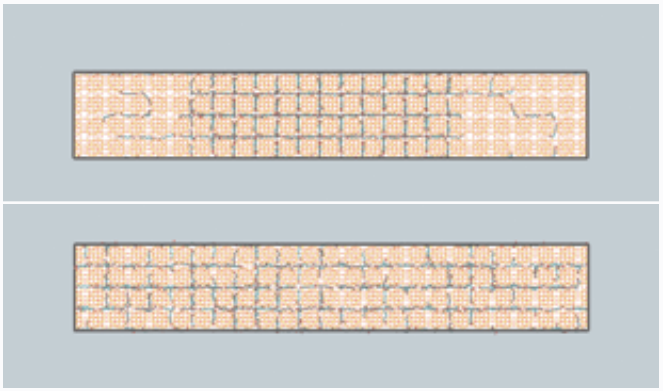
Bassman, L., A. Krishnamoorthy, H. Kumazoe, M. Misawa, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. "Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in $MoSe_2$ Monolayer," *Nano Letters* (July 2018), American Chemical Society.

Lin, M.-F., V. Kochat, A. Krishnamoorthy, L. Bassman, C. Weninger, Q. Zheng, X. Zhang, A. Apte, C. S. Tiwary, X. Shen, R. Li, R. Kalia, P. Ajayan, A. Nakano, P. Vashishta, F. Shimojo, X. Wang, D. Fritz, and U. Bergmann. "Ultrafast Non-Radiative Dynamics of Atomically Thin $MoSe_2$," *Nature Communications* (November 2017), Springer Nature.

Materials Science

Predictive Modeling of Functional Nanoporous Materials, Nanoparticle Assembly, and Reactive Systems

PI J. Ilja Siepmann
INST University of Minnesota
HOURS ALCC, 146 Million Core-Hours
(ALCF: 130M; NERSC: 16M)



Fluid-solid coexistence of adsorbed 1,5-pentanediol observed in a large supercell (consisting of 36 MFI unit cells) at **(A)** T = 323 K and **(B)** 383 K. The zig-zag channels run vertically and the straight channels run horizontally. *Image: Robert F. DeJaco and J. Ilja Siepmann, University of Minnesota*

Nanoporous materials, such as 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 selective catalysts. Finding an optimal material for a given application, however, is a time- and labor-intensive process that could take decades with traditional laboratory methods. This ALCC project takes advantage of ALCF computing resources to run simulations that help us better understand properties of certain nanoporous materials.

CHALLENGE Characterizing the adsorption processes of linear alkane-α, ω-diols (hereafter, referred to as diols) at elevated temperatures and pressures is important for the design of liquid adsorption systems, but it introduces experimental challenges with conventional equipment. Additionally, biomass-derived mixtures contain assorted molecules, many of which form hydrogen bonds with one another resulting in highly non-ideal solution behavior and leading to higher computational expense.

APPROACH In this ALCC project, the researchers employed large ensembles of molecular simulations with enhanced sampling techniques and adsorption experiments to obtain the binary adsorption equilibria of diols with 3-6 carbons from aqueous solution at T = 323 and 348 K and p = 1.0 bar. They used thermodynamics and quantitative structure analysis to explain the unique behavior of each diol in this homologous series confined in mordenite framework inverted.

RESULTS In a recent combined simulation and experiment paper in the *Journal of Chemical Physics*, the team detailed how they used Mira to run advanced Monte Carlo simulations and compute adsorption isotherms for diols. ALCF staff members assisted with setting up large ensemble calculations on both Mira and Theta. They observed good agreement between simulation and experiment for diols with fewer than six carbons and interesting effects from the framework structure observed for six carbons. Since the diols have been used to aid in the understanding of hydrogen-bonding behavior in solution of carbohydrates, they believe that this analysis may be quite informative for the adsorption mechanism of more complex polyols.

In addition, the research team has received a patent for their earlier work on Mira, involving the development of a process that uses zeolites for the separation of ethanol and water. One other patent application based on results obtained on Mira is pending.

IMPACT The diols investigated are high-value chemicals with many applications in the polymer and solvent industries, making their renewable production attractive. The systems and processes targeted in this project are of interest for the chemical, biorenewable, and petrochemical industries, and improving nanoporous materials for these applications has significant societal benefits.

PUBLICATIONS

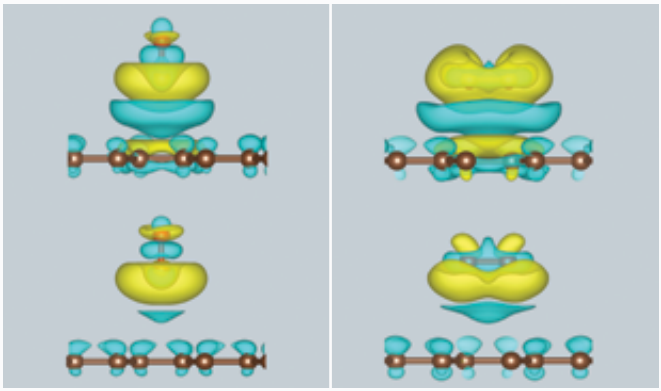
DeJaco, R. F., B. Elyassi, M. D. De Mello, N. Mittal, M. Tsapatsis, and J. I. Siepmann. "Understanding the Adsorption of Alkane-α, ω-Diols in Silicalite-1," *The Journal of Chemical Physics* (June 2018), American Institute of Physics.

Siepmann, J. I., P. Bai, and M. Tsapatsis. "Zeolites for Separation of Ethanol and Water," U.S. Patent, 10,039,999 (2018).

Materials Science

Predictive Simulations of Functional Materials

PI Paul Kent
INST Oak Ridge National Laboratory
HOURS INCITE, 140 Million Core-Hours
(ALCF: 100M; OLCF: 40M)



Side view of the total electron density difference between 2 van der Waals corrected DFT functionals for **(A)** V-mode and **(B)** A-mode at a distance of (top) 2.6 \AA and (bottom) 3.4 \AA. *Image: Anouar Benali, Argonne National Laboratory; Yongkyung Kwon and Hyeondeok Shin, Konkuk University*

Recent advances in Quantum Monte Carlo (QCM) methods promise to expand functional materials development, the possibilities of which have been greatly hindered by the limited predictive powers of traditional quantum mechanics-based approaches. A research team led by Oak Ridge National Laboratory has been using simulations made possible by DOE supercomputers to study the remarkable properties of the substance graphene, a material which stands to revolutionize an array of applications through the creation of faster transistors and electronic components.

CHALLENGE Since its successful isolation in 2004, monolayer graphene has been an object of intense research interest. Its many remarkable properties include Dirac cones, electronic band structures that describe unusual (and beneficial) electron transport. Monolayer graphene consists of a single layer of atoms (and is hence referred to as a two-dimensional material), the bonding structure of whose electron orbitals makes it extremely susceptible to environmental perturbation. Oxygen, due to its abundance and interactivity, is among the most important potential contaminants to study in depth.

APPROACH In its study the team worked with QMCPACK, a QMC code written specifically for high-performance computers and used at the ALCF since 2011.

QMC approaches solve the quantum many-body problem stochastically. They offer three key advantages over traditional density functional theories (DFT): accuracy, efficiency, and, with only three possible sources of error, transparency. Moreover, they establish a strict upper-bound for total energy and exactly compute interatomic and -molecular interactions known as van der Waals forces, which DFT approaches can only approximate. As such, the exceptional power of QMC made it ideal for modeling adsorption and diffusion of oxygen molecules on graphene surfaces.

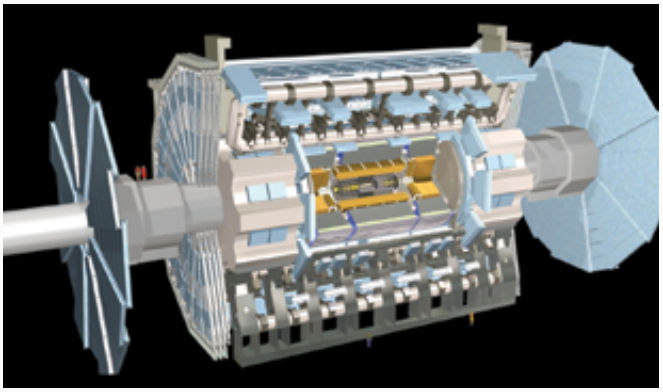
RESULTS Using simulations on Mira to examine various orientations of oxygen on the surface of graphene, the team was able to identify the most energetically stable modes. Furthermore, the results exposed the appreciable bias of DFT functionals toward under- and overestimations that van der Waals corrections entail.

IMPACT This work, by identifying stable oxygen energy modes with an accuracy unachievable without the use of high-performance computers, brings graphene closer to industrial application once it can be produced on appropriate scales. As its features can lead to significantly faster transistors and electronic components, graphene offers substantial promise.

Physics

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

PI Taylor Childers
INST Argonne National Laboratory
HOURS ADSP, 45 Million Core-Hours



A cut-away diagram of the ATLAS detector, which stands at 82 feet tall and 144 feet long. Protons enter the detector from each side and collide in the center. *Image: ATLAS/CERN*

CERN's Large Hadron Collider (LHC) produces more data than it can analyze, and that amount is only increasing. When CERN upgrades to the High-Luminosity LHC in 2026, experimental data produced are expected to increase by a factor of 10. To help meet the LHC's growing computer needs, a research team is putting ALCF supercomputers to work simulating LHC collisions and optimizing these algorithms which were written for traditional computing resources.

CHALLENGE With the ADSP allocation, the team is addressing the communication and data flow challenges that come with using leadership scale supercomputers like Theta. Unlike traditional computing resources, like those on the Worldwide LHC Computing Grid, Theta requires highly-parallel workflows with inter-node orchestration. Without these workflows, it is difficult to effectively fill the available CPU resources at all HPC centers without manual intervention.

APPROACH The team has developed an edge service called Harvester that retrieves ATLAS production jobs from the global servers at CERN, stages the proper data to the local shared file system, and launches the batch job to execute the ATLAS analysis. On systems with no outbound connectivity on the compute node, like Theta, Harvester can handle the communication on the login-nodes. The team also developed Yoda, an MPI-enabled wrapper for the ATLAS analysis framework that runs on Theta.

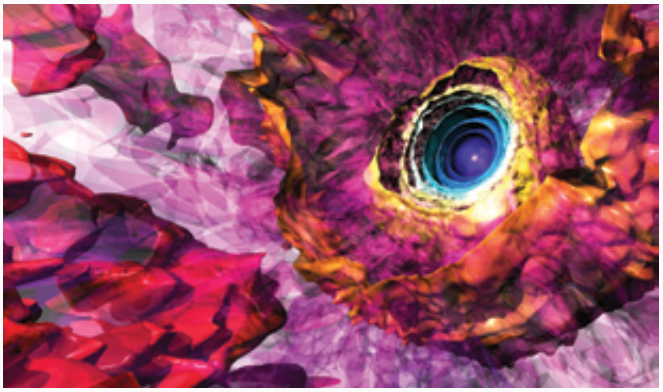
RESULTS Harvester and Yoda are being integrated into the ATLAS production system, called PanDA, to run the ATLAS analysis framework on Theta. The ATLAS simulation process is composed of three steps—event generation, simulation, and reconstruction—but so far only simulation has been run on Theta using the production system. The workflow is being tested on Theta and has simulated over 12 million collision events. The team continues to optimize the other two steps for ALCF resources.

IMPACT This project is increasing the scientific reach of LHC experiments to probe the fundamental forces and particles that make up the universe. High-precision measurements will be the driver of discovery in the next 10 years of LHC physics analyses, and ALCF computing resources will be essential for success. In addition, technologies developed to help the LHC advance science can be used in other big data applications.

Physics

Global Radiation MHD Simulations of Massive Star Envelopes

PI Lars Bildsten
INST University of California, Santa Barbara
HOURS INCITE, 60 Million Core-Hours



Global radiation hydrodynamic simulation of massive star envelope. *Image: Joseph A. Insley, Argonne National Laboratory*

Massive stars play an important role in many astrophysical environments, but poor understanding of mass loss creates uncertainties in our knowledge of their evolution. Winds from these stars depend on their surface layer structure, including the effects of instabilities that can only be understood through large-scale 3D simulations. A team of University of California, Santa Barbara researchers is using such simulations to study the global structure of the gaseous outer layers, or envelopes, of massive stars.

CHALLENGE The most important modes of stellar mass loss (which decisively affect the evolution and final fate of massive stars) are still the most uncertain, hindering the predictive power of evolutionary models and necessitating quantitative studies of the stability of radiation-dominated star envelopes and its role in stellar mass loss at different levels of metallicity. The researchers therefore aim to study the global structure of massive star envelopes by examining different stellar masses and evolutionary stages via 3D radiation magnetohydrodynamic (MHD) simulations. The simulations capture the global properties of the star and wind while resolving the structure of the stellar atmosphere.

APPROACH With Mira's computational power the researchers are able to run the grid-based code Athena++ to solve the ideal MHD equation with time-dependent radiative transfer. The calculations solve for true 3D structure of the atmosphere and wind of a massive star given its mass and age.

RESULTS The researchers repeated two of the first year's global simulations with different metallicities to study the effects thereof on envelope structures and mass-loss rate, detailing their findings in *Nature*. It was discovered that increased metallicity produces stronger turbulence and causes a larger helium opacity peak, leading to stronger winds and larger amplitude variability. Reduced metallicity fails to produce a strong helium opacity peak, reducing the outflow rate from massive stars.

IMPACT By answering long-standing questions about the properties of powerful winds from massive stars, this work will dramatically improve our understanding of the surface layers of massive stars and benefit the astrophysics community. The results will be incorporated into one-dimensional stellar evolution models to create more realistic massive star models, significantly advancing our knowledge of their structure and evolution, and lead to more accurate pre-supernova progenitor models for use in simulations of core-collapse supernovae.

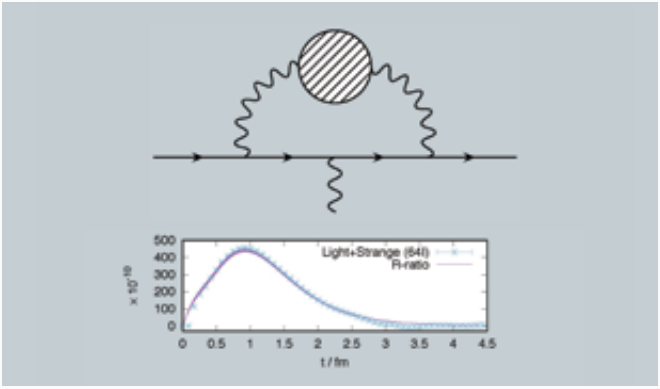
PUBLICATIONS

Jiang, Y.-F., M. Cantiello, L. Bildsten, E. Quataert, O. Blaes, and J. Stone. "Outbursts of Luminous Blue Variable Stars from Variations in the Helium Opacity," *Nature* (September 2018), Springer Nature.

Physics

Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment

PI Thomas Blum
INST University of Connecticut
HOURS ALCC, 220 Million Core-Hours



Hadronic vacuum polarization contribution to the muon anomaly. Left: muon (horizontal line) interacting with hadrons (shaded loop) through emission of virtual photons (upper wavy lines). Right: contribution to the anomaly (crosses) with distance between the virtual photons in femtometers. *Image: Thomas Blum, University of Connecticut*

The Standard Model has been the definitive description of particle physics in the past 50 years, but it's being challenged by a discrepancy between the measured and predicted values of the magnetic moment of a particle called the muon. This project aims to quantify and reduce the largest uncertainties associated with this value in order to obtain the most precise calculation of the anomaly. These results, combined with data soon to come from Fermilab's Muon g-2 experiment, may lead to the discovery of new physics beyond the Standard Model.

CHALLENGE The muon's magnetic moment describes how this fundamental particle interacts with a magnetic field; it depends on all particles that can couple to the muon—including as-yet-undiscovered particles. The muon moment has been both measured in experiments and calculated theoretically, but those two values don't quite match up—hinting at the existence of new physics. A higher-precision measurement could erase the discrepancy, so minimizing uncertainties in the theoretical calculation is necessary to reach a more definite conclusion. The largest uncertainty in the calculation comes from particles that interact through the strong force, known as hadronic contributions. Since these contributions can't be solved with conventional perturbative methods at low-energy scales, researchers previously resorted to experimental data or approximations with large uncertainties.

APPROACH The team used lattice quantum chromodynamics (QCD) to compute the hadronic contributions by allowing particles to exist only on a discrete lattice. They used Mira to solve the complex mathematical equations of QCD, which encode all possible strong interactions with the muon.

RESULTS In a paper recently published in *Physical Review Letters*, the team detailed their successful determination of the most precise prediction of the leading-order hadronic vacuum polarization contribution to the muon's magnetic moment. An earlier result published by the team in *Physical Review Letters* reported the first-ever calculation of the sub-leading hadronic light-by-light contribution with physical masses, also computed on Mira. Ongoing calculations on Mira will remove and reduce systematic and statistical errors of these results.

IMPACT These results have led to a more precise calculation of the muon magnetic moment. Once experimental measurements from Fermilab's Muon g-2 experiment come out in 2019, the two values can be compared, potentially leading to the discovery of new physics.

PUBLICATIONS

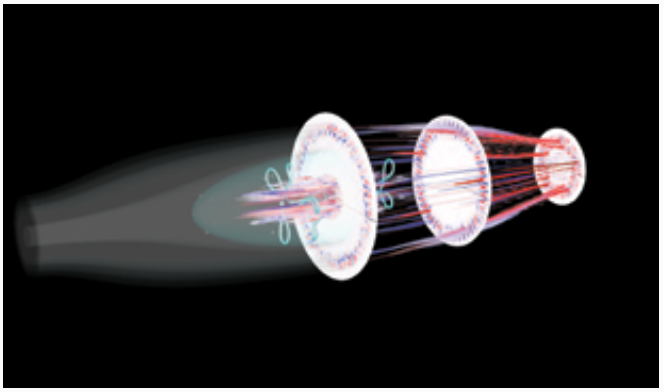
Blum, T., N. H. Christ, M. Hayakawa, T. Izubuchi, L. Jin, C. Jung, and C. Lehner. "Connected and Leading Disconnected Hadronic Light-by-Light Contribution to the Muon Anomalous Magnetic Moment with a Physical Pion Mass," *Physical Review Letters* (January 2017), American Physical Society.

Blum, T., P. A. Boyle, V. Gülpers, T. Izubuchi, L. Jin, C. Jung, A. Jüttner, C. Lehner, A. Portelli, and J. T. Tsang. "Calculation of the Hadronic Vacuum Polarization Contribution to the Muon Anomalous Magnetic Moment," *Physical Review Letters* (July 2018), American Physical Society.

Physics

Kinetic Simulation of FRC Stability and Transport

PI Sean Dettrick
INST TAE Technologies Inc.
HOURS INCITE, 30 Million Core-Hours



3D simulations of micro-turbulence in the field reversed configuration, performed using the ANC code on Theta. Red and blue streamers represent perturbations to the electrostatic potential, also shown in three cross sections as color density plots. The meandering light blue curve shows a typical large ion orbit in the FRC. *Image: Daniel Fulton, Kevin Hubbard, and Calvin Lau, TAE Technologies, Inc.*

Fusion energy offers the prospect of a carbon-neutral, environmentally responsible, and inexhaustible energy source. Researchers from TAE Technologies Inc. are using ALCF computing resources to accelerate their fusion plasma research program aimed at developing the world's first commercially viable fusion-powered generator for electricity production.

CHALLENGE The central challenge in generating fusion energy for commercial use is to keep plasma hot enough for long enough to sustain the fusion reaction. TAE Technologies has built "Norman," an advanced beam-driven field-reversed configuration (FRC) plasma device, for experimental studies of the magnetic confinement of hot fusion plasmas. Heat can be lost from the FRC due to nonlinear wave-particle interactions, which start at the microscale and lead to kinetic turbulence. On the macroscale, nonlinear wave-particle interactions can also determine the global stability of the plasma.

APPROACH To understand both the microscale and macroscale kinetic plasma physics of the FRC, the research team is using Theta to develop the ANC kinetic micro-turbulence code and the FPIC kinetic macro-stability code to enable massively parallel 3D particle-in-cell (PIC) simulations of the Norman experiment. The ANC code, developed in collaboration with the University of California, Irvine, will be used to interpret experimental measurements of turbulence and to understand how heat loss (transport) scales with plasma temperature. The FPIC code will be used to help understand the global stability and self-organization of the plasma, and to inform the feedback and control strategies that will be used on Norman.

RESULTS The TAE team has made a number of physics model advances and numerical algorithm improvements with the two codes. This work has allowed them to increase physics understanding by comparing experimentally measured and computationally simulated FRC turbulence for the first time. The researchers have also developed theoretical stability models suggested by the results of FPIC global stability simulations. The combination of these developments, and the validation of the codes against the Norman experiment, will enable TAE Technologies to perform predictive simulations of transport and stability in FRC plasmas.

IMPACT This project will help accelerate TAE Technologies' studies of the confinement of energy with high plasma temperatures and inform the design of a future prototype reactor. If the company's technology can be extended to fusion-relevant temperatures, it will provide an economical path to clean, safe, and sustainable fusion energy.

Lattice QCD

PI Paul Mackenzie
INST Fermilab
HOURS INCITE, 444 Million Core-Hours
(ALCF: 344M; OLCF: 100M)

An antiquark (magenta) inside a cloud of gluons (green). USQCD researchers discovered a new and unambiguous way to decide how much of the cloud's energy should be considered part of the quark mass. This idea was applied to simulation data generated with Mira to compute quark massed from first principles. *Image: Joseph A. Insley, Argonne National Laboratory*

Accurate measurements of quark masses are necessary to develop precise predictions about the Standard Model. In this INCITE project, researchers from the U.S. Lattice Quantum Chromodynamics (USQCD) Collaboration are using ALCF computing resources to perform calculations of the up-, down-, strange-, charm-, and bottom-quark masses. These calculations provide critical input to experimental searches for new physics beyond the Standard Model.

CHALLENGE Atomic nuclei are composed of subatomic particles called protons and neutrons, which are themselves composed of fundamental particles called quarks. While protons and neutrons get most of their mass from the force that binds the quarks together, the quark masses themselves also contribute, ranging from the light up and down quarks that make up protons to the heavy top quark 185 times more massive than a proton. To determine these mass values, scientists must compare theoretical calculations of an appropriate set of observables to experimental measurements of those observables.

APPROACH This ongoing project uses DOE leadership computing resources to advance research in QCD (the theory of the strong interaction between quarks and gluons). Using lattice QCD, a non-perturbative approach to QCD, the team is able to calculate the observables required to determine quark masses. The researchers also developed a new heavy-quark effective theory (HQET)-based method to extract quark masses from the masses of bound states of a light quark with a heavy quark. ALCF staff helped optimize the MILC code for Mira, including improving communications performance and adding vector math instructions.

RESULTS Using lattice QCD and the HQET-based method on Mira, the researchers found the charm-, and bottom-quark masses, as well as quark mass ratios yielding the up-, down-, strange-quark masses. The charm quark mass they determined matches the most precise result to date, and the other masses and all ratios are the most precise to date. Thus, the new HQET-based method proved to be successful quantitatively as well as qualitatively.

IMPACT Making accurate determinations of quark masses is important to understanding whether their mass originates from interactions with the recently discovered Higgs field, as is currently expected. This project is also carrying out precise lattice QCD calculations to address key science questions in particle and nuclear physics and to support corresponding experimental programs, such as the Muon g-2 experiment at Fermilab and the GlueX experiment at Jefferson Lab.

PUBLICATIONS

Brambilla, N., J. Komijani, A. S. Kronfeld, and A. Vairo. "Relations Between Heavy-Light Meson and Quark Masses." *Physical Review D* (February 2018), American Physical Society.

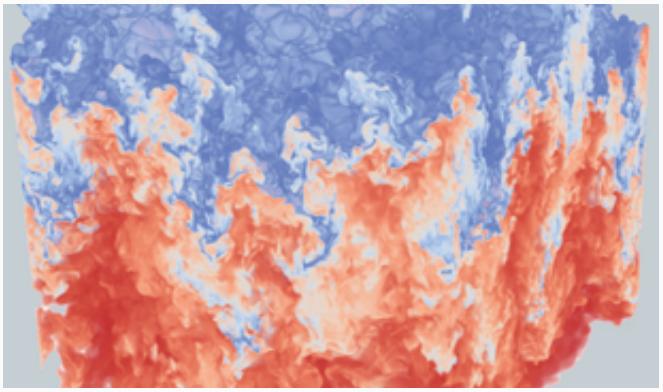
Bazavov, A., et al. "Up-, Down-, Strange-, Charm-, and Bottom-Quark Masses from Four-Flavor Lattice QCD." *Physical Review D* (September 2018), American Physical Society.

Bazavov, A., et al. "B- and D-meson Leptonic Decay Constants from Four-Flavor Lattice QCD." *Physical Review D* (accepted), American Physical Society.

Physics

Multiscale Physics of the Ablative Rayleigh-Taylor Instability

PI Hussein Aluie
INST University of Rochester
HOURS INCITE, 90 Million Core-Hours



Grand-challenge fully compressible Rayleigh-Taylor simulation carried out at an unprecedented resolution of 1,024 x 1,024 x 2,048 grid points. Image: Dongxiao Zhao, University of Rochester

Rayleigh-Taylor Instability (RTI), a ubiquitous phenomenon that occurs when a heavy fluid is accelerated against a light fluid, is a major obstacle to current efforts to realize inertial confinement fusion as an energy source. Researchers from the University of Rochester are using ALCF resources to study, via simulations, how ablation (mass evaporation due to a heat source) affects RTI evolution. In doing so they hope to elucidate RTI's role in internal confinement fusion implosions.

CHALLENGE RTI, which has hindered yields in internal confinement fusion, describes the interfacial instability of a dense fluid atop a lighter fluid when a downward acceleration field is present. It can be viewed as a given system's attempt to reduce its potential energy by lowering its center of mass, manifested in the formation of rising bubbles and sinking spikes in the light and heavy fluids, respectively. Such flows further amplify fluctuations and mixing, which leads to extreme nonlinearity.

With a variety of simulations, the researchers aim to determine the effect of ablation on RTI and how to model ablative RTI when including nonlinear instabilities. A major difficulty in numerically modeling flow systems exhibiting RTI is the vast range of scales involved, all of which are dynamically coupled due to the flow's highly nonlinear nature.

APPROACH The researchers used Mira to run high-resolution simulations generated by DiNuSUR, a hybrid spectral, compact-finite-difference code they developed. DiNuSUR can simulate compressible and incompressible fluid flows, and the evolution of tracers passively advected by the flow. It also features modules to solve a host of equations, including Navier-Stokes, Boussinesq, and magnetohydrodynamic equations. A Fortran 2003 MPI code, DiNuSUR demonstrates excellent parallelism, having scaled to one sixth of the Mira system (roughly 130,000 cores) for the largest simulations.

RESULTS The researchers discovered that, contrary to current modeling practices, any length-scale in ablative RTI can be destabilized if the initial perturbation is sufficiently large. The vast dynamic range afforded by their simulations provided numerical evidence for the optimal way to analyze length-scales in highly nonlinear flows with significant density variations. The team detailed these findings in a paper published in *Physical Review E*.

IMPACT Beyond bringing nuclear fusion closer to realization as a viable and virtually limitless energy source, this work carries important ramifications for modeling implosion physics, astrophysics, oceanic flows, and combustion science.

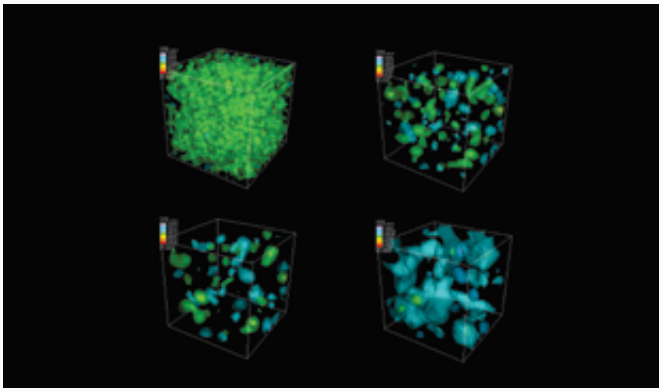
PUBLICATIONS

Zhang, H., R. Betti, V. Gopalaswamy, R. Yan, and H. Aluie. "Nonlinear Excitation of the Ablative Rayleigh-Taylor Instability for All Wave Numbers," *Physical Review E* (January 2018), American Physical Society.

Physics

Nucleon Structure and Electric Dipole Moments with Physical Chirally-Symmetric Quarks

PI Sergey Syritsyn
INST RIKEN BNL Research Center
HOURS ALCC, 50 Million Core-Hours



Topological charge in QCD vacuum (inducing EDM in the nucleon) *Image: Sergey Syritsyn, RIKEN BNL Research Center*

A predominant goal in contemporary nuclear physics is understanding how strong interaction of quarks and gluons creates the rich structure of nuclear matter. By utilizing ALCF resources to perform their calculations, a team from the RIKEN BNL Research Center and Stony Brook University is attempting to realize this goal—that is, to answer the underlying question of how subatomic matter organizes itself.

CHALLENGE High-precision nuclear physics is a vital component of searches for new physics that manifest in violations of fundamental symmetries. In particular, observation of permanent electric dipole moments (EDMs) of nucleons and nuclei would be direct evidence for violation of CP (charge conjugation and parity) symmetry. Developing our understanding of the quantitative connection between EDM magnitudes and CP violations at the quark-gluon level will reduce the theoretical gap to arise from near-future experiments (thereby enabling more correct interpretation of the resulting data), while precise data on nucleon axial form factors will soon be needed to correctly measure neutrino flux.

The calculations done here will incorporate state-of-the-art features from lattice quantum chromodynamics (QCD), including quarks with physical masses, an improved quark discretization, and new gauge ensembles.

APPROACH To perform their work, the researchers have been running the software suite Qlua on Mira. This production code is a lattice QCD domain-specific language that incorporates solvers, science-related algebra primitives, and I/O. Python is the main instrument for post-analysis.

Notably, the transverse momentum dependent (TMD) calculation included in the INCITE project "Hadron Structure from Lattice QCD" has been successfully integrated with this work. The calculation scheme was so efficient that the calculation was extended to additional nucleon structure observables.

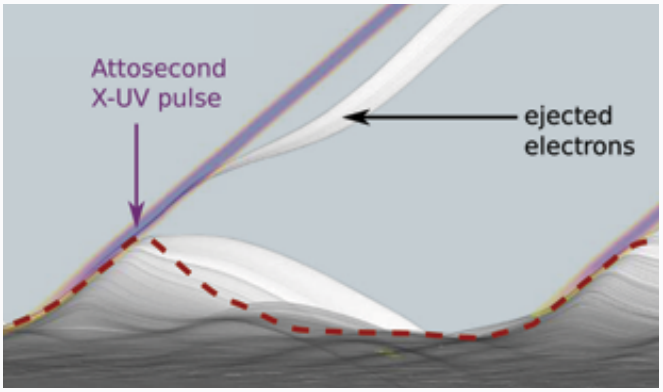
RESULTS Generating 33,000 samples, the researchers have continued to accumulate statistics for primary observables (i.e., nucleon form factors and electric dipole moments). These statistics are expected to reduce the error bars for form factors and the neutron EDM even further. Additionally, nonperturbative renormalization calculations are underway for CP-odd quark-gluon operators.

IMPACT Precise calculations of nucleon structure help advance the DOE mission in many ways. The predictions they provide will help determine nucleon features such as form factors and structure functions, and quark and gluon contributions to proton spin. Furthermore, this work will inform strategic decisions concerning the design of Brookhaven's future Electron-Ion Collider.

Physics

PICSSAR: Particle-In-Cell Spectral Scalable Accurate Relativistic

PI Jean-Luc Vay, Henri Vincenti
INST Lawrence Berkeley National Laboratory, CEA Saclay, France
HOURS INCITE, 89 Million Core-Hours *(ALCF: 80M; OLCF: 9M)*



A plasma mirror exposed to a UHI laser field with plasma electron density (gray color map), vacuum (white), and emitted attosecond light pulses (violet). The relativistic electron bunches ejected into the vacuum appear in gray. *Image: Henri Vincenti, CEA Saclay, France*

To explore the new and promising—yet still largely unexplored—field of ultra-high intensity physics (UHI), researchers need highly accurate particle-in-cell (PIC) modeling capabilities. This INCITE project combines the computing power of Mira with the precision and scalability of the team's new pseudo-spectral PIC code to enable, for the first time, the realistic 3D modeling of novel compact particle and light sources generated on plasma mirrors. Their new method will be vital to the advancement of ultrafast science and high energy physics.

CHALLENGE The rise of UHI physics has been spurred by the advent of high power petawatt femtosecond lasers. When this laser is focused on a solid target, the intensity can reach values at which matter is fully ionized and turns into a dense plasma that can reflect incident light—a "plasma mirror." This mirror can produce promising sources of high-charge relativistic electrons and X-UV attosecond radiation sources. Further exploration of the physics of plasma mirrors requires PIC modeling at accuracies unattainable with standard PIC codes that use the finite-difference time domain (FDTD) method to solve Maxwell's equations.

APPROACH Researchers are now using ultrahigh-order pseudo-spectral Fast Fourier Transform (FFT)-based methods—which offer several advantages over standard FDTD solvers in terms of accuracy and stability. FFT-based methods have previously been problematic because of their poor scalability, so a pioneering grid decomposition technique was recently implemented in the team's PIC code Warp+PXR. ALCF staff helped the team overcome job scripting issues facilitating parameter scans on Mira and Cooley.

RESULTS Using Mira, the researchers showed that the new technique scales up to a million cores and therefore can handle these complex 3D simulations. This modeling has been used to interpret experiments performed at CEA Saclay and elucidate an important laser absorption mechanism in dense plasmas. The team recently published a paper detailing the new FFT-based method in *Computer Physics Communications* and submitted a paper on laser absorption in dense plasmas in *Physical Review X*.

IMPACT This project is performing simulations that will help researchers design, optimize, and control the next generation of particle and light sources produced by UHI laser interactions on plasma mirrors. These sources can be applied to medicine, industry, and other fields of research, including high energy physics and ultrafast science.

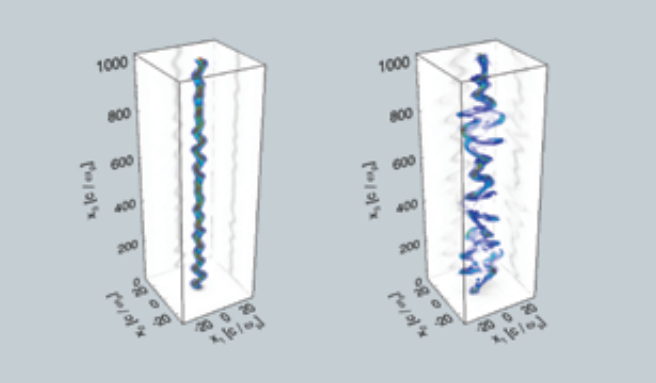
PUBLICATIONS

Vincenti, H. and J.-L. Vay. "Ultrahigh-Order Maxwell Solver with Extreme Scalability for Electromagnetic PIC Simulations of Plasmas," *Computer Physics Communications* (July 2018), Elsevier.

Physics

Studying Astrophysical Particle Acceleration in HED Plasmas

PI Frederico Fiuza
INST SLAC National Accelerator Laboratory
HOURS ALCC, 50 Million Core-Hours



Simulated disruption of current filaments in a plasma. Current filaments produced during the interaction of counter-streaming plasmas are unstable to a kink mode. Radial deformation of the filament leads to disruption of the current and isotropization of the magnetic field, causing slow down of the plasma flows and the formation of a collisionless shock. *Image: Frederico Fiuza, SLAC National Accelerator Laboratory*

The origin of cosmic rays and their dominant acceleration mechanisms (and whether these mechanisms are laboratory-reproducible) remain open, fascinating problems in science, problems closely tied to fundamental processes—collisionless shocks, magnetic reconnection, and turbulence—associated with particle acceleration in high-energy-density (HED) plasma environments. Researchers from the SLAC National Accelerator Laboratory are harnessing ALCF supercomputers to run simulations of these processes that open the door for future laboratory experiments, potentially leading to transformative advances in our understanding of physics.

CHALLENGE The researchers are using 3D, massively parallel particle-in-cell (PIC) simulations to explore the physics of particle acceleration and magnetic field dynamics in HED plasmas. In particular, based on laser-ablated plasma profiles obtained from HYDRA simulations at the National Ignition Facility (NIF), the team wants to characterize the formation of collisionless shocks and study particle injection that occurs during these shocks. This research will guide design and interpretation of future NIF laser experiments.

APPROACH The researchers are using Mira to run OSIRIS, a fully explicit, fully parallelized, fully relativistic, electromagnetic, and object-oriented particle-in-cell code (PIC) written in Fortran 90 using MPI and HDF5. OSIRIS has recently been complemented with the extension h-OSIRIS for multiscale collisional and collisionless plasma simulations, smoothly coupling the smaller electromagnetic kinetic scales and the larger fluid/hybrid scales, thereby resolving a longstanding problem.

RESULTS As HYDRA simulations optimizing flow density and velocity near the interaction region are now complete, the researchers have performed PIC simulations based on the ensuing profiles. Their results indicate the possibility of observing strong compression associated with collisionless shock formation.

The researchers also explored particle injection in collisionless shocks for different plasma conditions using data obtained from HYDRA, discovering that particles develop a non-thermal tail at the time of shock formation. The team subsequently characterized the electron and ion spectra as functions of time, and will use these results to inform selection of experimental diagnostics.

IMPACT Aside from expanding our basic understanding of the universe, particle accelerator studies significantly impact the generation of new laboratory accelerators for a variety of applications, ranging from fusion plasma diagnostics to medical imaging. By elucidating particle acceleration in high energy density plasmas, this project is important to the DOE's Frontiers of Plasma Science Program. Furthermore, it dramatically advances our ability to model magnetic field dynamics and particle injection in laboratory and astrophysical plasmas.

ALCF Projects

2018 INCITE Projects

Biological Sciences

Biophysical Principles of Functional Synaptic Plasticity in the Neocortex

PI Eilif Muller, Blue Brain Project
INST EPFL
HOURS 160 Million Core-Hours

The Free Energy Landscapes Governing Membrane Protein Function

PI Benoît Roux
INST The University of Chicago
HOURS 92 Million Core-Hours

Finite Difference Time Domain Simulations to Facilitate Early-Stage Human Cancer Detection

PI Allen Taflove
INST Northwestern University
HOURS 80 Million Core-Hours

Chemistry

Advancing Design and Structure Prediction of Proteins and Peptides

PI David Baker
INST University of Washington
HOURS 120 Million Core-Hours

High-Accuracy Quantum Approaches for Predictions of Catalysis on Solids

PI Maria Chan
INST Argonne National Laboratory
HOURS 47 Million Core-Hours
(ALCF: 42M; OLCF: 5M)

Computer Science

Performance Evaluation and Analysis Consortium (PEAC) End Station

PI Leonid Oliker
INST Lawrence Berkeley National Laboratory
HOURS 89 Million Core-Hours
ALCF: 54M; OLCF: 35M

Earth Science

Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations

PI Thomas H. Jordan
INST University of Southern California
HOURS 126 Million Core-Hours
ALCF: 30M; OLCF: 96M

High-Resolution Climate Change Simulations with the CESM

PI Gerald Meehl
INST NCAR
HOURS 264 Million Core-Hours

Accelerated Climate Modeling for Energy (ACME)

PI Mark Taylor
INST Sandia National Laboratories
HOURS 179 Million Core-Hours
ALCF: 89M; OLCF: 90M

Energy Technologies

Towards Predictive Exascale Wind Farm Simulations

PI Michael Sprague
INST NREL
HOURS 115 Million Core-Hours
ALCF: 110M; OLCF: 5M

Engineering

Multiscale Physics of the Ablative Rayleigh-Taylor Instability

PI Hussein Aluie
INST University of Rochester
HOURS 90 Million Core-Hours

Crystal Plasticity from First Principles

PI Vasily Bulatov
INST Lawrence Livermore National Laboratory
HOURS 110 Million Core-Hours

Adaptive DDES of a Vertical Tail/Rudder Assembly with Active Flow Control

PI Kenneth Jansen
INST University of Colorado Boulder
HOURS 207 Million Core-Hours

High-Accuracy LES of a Multistage Compressor Using Discontinuous Galerkin

PI Koen Hillewaert
INST Cenaero
HOURS 78 Million Core-Hours

Large-Eddy Simulation of a Commercial Transport Aircraft Model

PI Parviz Moin
INST Stanford University
HOURS 240 Million Core-Hours

Large-Eddy Simulation for the Prediction and Control of Impinging Jet Noise

PI Joseph Nichols
INST University of Minnesota
HOURS 81 Million Core-Hours

Convective Turbulence in Liquid Sodium

PI Janet Scheel
INST Occidental College
HOURS 80 Million Core-Hours

Materials Science

Modeling Electronic Stopping in Condensed Matter Under Ion Irradiation

PI Yosuke Kanai
INST University of North Carolina at Chapel Hill
HOURS 155 Million Core-Hours

Predictive Simulations of Functional Materials

PI Paul Kent
INST Oak Ridge National Laboratory
HOURS 140 Million Core-Hours
ALCF: 100M; OLCF: 40M

Materials and Interfaces for Organic and Hybrid Photovoltaics

PI Noa Marom
INST Carnegie Mellon University
HOURS 260 Million Core-Hours

Petascale Simulations for Layered Materials Genome

PI Aiichiro Nakano
INST University of Southern California
HOURS 200 Million Core-Hours

Physics

Global Radiation MHD Simulations of Massive Star Envelopes

PI Lars Bildsten
INST University of California, Santa Barbara
HOURS 60 Million Core-Hours

Collider Physics at the Precision Frontier

PI Radja Boughezal
INST Argonne National Laboratory
HOURS 98 Million Core-Hours

High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics

PI C.S. Chang
INST Princeton Plasma Physics Laboratory
HOURS 162 Million Core-Hours
ALCF: 62M; OLCF: 100M

Extreme-Scale Simulation of Supernovae and Magnetars from Realistic Progenitors

PI Sean Couch
INST Michigan State University
HOURS 159 Million Core-Hours

Multiscale Modeling of Magnetic Reconnection in Space and Laboratory Plasmas

PI William Daughton
INST Los Alamos National Laboratory
HOURS 24 Million Core-Hours

Kinetic Simulation of FRC Stability and Transport

PI Sean Dettrick
INST TAE Technologies, Inc
HOURS 30 Million Core-Hours

Nuclear Structure and Nuclear Reactions

PI Gaute Hagen
INST Oak Ridge National Laboratory
HOURS 180 Million Core-Hours
ALCF: 100M; OLCF: 80M

Lattice QCD

PI Paul Mackenzie
INST Fermilab
HOURS 444 Million Core-Hours
ALCF: 344M; OLCF: 100M

Hadron Structure from Lattice QCD

PI Konstantinos Orginos
INST College of William & Mary
HOURS 155 Million Core-Hours
ALCF: 55M; OLCF: 100M

PICSSAR

PI Jean-Luc Vay
INST Lawrence Berkeley National Laboratory
HOURS 88 Million Core-Hours

Astrophysical Particle Accelerators: Magnetic Reconnection and Turbulence

PI Dmitri Uzdensky
INST University of Colorado
HOURS 98 Million Core-Hours

2017–2018 ALCC Projects

Biological Sciences

Multiscale Simulations of Hematological Disorders

PI George Karniadakis
INST Brown University
HOURS 46 Million Core-Hours
ALCF: 20M; OLCF: 26M

Protein-Protein Recognition and HPC Infrastructure

PI Benoît Roux
INST The University of Chicago
HOURS 80 Million Core-Hours

Chemistry

Quantum Monte Carlo Computations of Chemical Systems

PI Olle Heinonen
INST Argonne National Laboratory
HOURS 5 Million Core-Hours

Spin-Forbidden Catalysis on Metal-Sulfur Proteins

PI Sergey Varganov
INST University of Nevada, Reno
HOURS 42 Million Core-Hours

Computer Science

ECP Consortium for Exascale Computing

PI Paul Messina
INST Argonne National Laboratory
HOURS 969 Million Core-Hours
ALCF: 530M; OLCF: 300M; NERSC: 139M

Portable Application Development for Next-Generation Supercomputer Architectures

PI Tjerk Straatsma
INST Oak Ridge National Laboratory
HOURS 60 Million Core-Hours
ALCF: 20M; OLCF: 20M; NERSC: 20M

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications

PI Robert Voigt
INST Leidos
HOURS 157 Million Core-Hours
ALCF: 110M; OLCF: 47M

Earth Science

Large-Eddy Simulation Component of the Mesoscale Convective System Climate Model Development and Validation (CMDV-MCS) Project

PI William Gustafson
INST Pacific Northwest National Laboratory
HOURS 74 Million Core-Hours

Understanding the Role of Ice Shelf-Ocean Interactions in a Changing Global Climate

PI Mark Petersen
INST Los Alamos National Laboratory
HOURS 87 Million Core-Hours
ALCF: 25M; OLCF: 2M; NERSC: 60M

Energy Technologies

High-Fidelity Numerical Simulation of Wire-Wrapped Fuel Assemblies

PI Elia Merzari
INST Argonne National Laboratory
HOURS 85 Million Core-Hours

Elimination of Modeling Uncertainties Through High-Fidelity Multiphysics Simulation to Improve Nuclear Reactor Safety and Economics

PI Emily Shemon
INST Argonne National Laboratory
HOURS 44 Million Core-Hours

Engineering

Non-Boussinesq Effects on Buoyancy-Driven Variable Density Turbulence

PI Daniel Livescu
INST Los Alamos National Laboratory
HOURS 60 Million Core-Hours

Numerical Simulation of Turbulent Flows in Advanced Steam Generators—Year 3

PI Aleksandr Obabko
INST Argonne National Laboratory
HOURS 50 Million Core-Hours

Materials Science

Computational Engineering of Electron-Vibration Coupling Mechanisms

PI Marco Govoni
INST The University of Chicago
Argonne National Laboratory
HOURS 75 Million Core-Hours
ALCF: 60M; NERSC: 15M

Imaging Transient Structures in Heterogeneous Nanoclusters in Intense X-Ray Pulses

PI Phay Ho
INST Argonne National Laboratory
HOURS 68 Million Core-Hours

Predictive Modeling of Functional Nanoporous Materials, Nanoparticle Assembly, and Reactive Systems

PI J. Ilja Siepmann
INST University of Minnesota
HOURS 146 Million Core-Hours
ALCF: 130M; NERSC: 16M

Modeling Helium-Hydrogen Plasma Mediated Tungsten Surface Response to Predict Fusion Plasma Facing Component Performance

PI Brian Wirth
INST Oak Ridge National Laboratory
HOURS 173 Million Core-Hours
ALCF: 98M; OLCF: 75M

Physics

Hadronic Light-by-Light Scattering and Vacuum Polarization Contributions to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions

PI Thomas Blum
INST University of Connecticut
HOURS 220 Million Core-Hours

High-Fidelity Gyrokinetic Study of Divertor Heat-Flux Width and Pedestal Structure

PI Choong-Seock Chang
INST Princeton Plasma Physics Laboratory
HOURS 270 Million Core-Hours
ALCF: 80M; OLCF: 100M; NERSC: 90M

Simulating Particle Interactions and the Resulting Detector Response at the LHC and Fermilab

PI Taylor Childers
INST Argonne National Laboratory
HOURS 188 Million Core-Hours
ALCF: 58M; OLCF: 80M; NERSC: 50M

Studying Astrophysical Particle Acceleration in HED Plasmas

PI Frederico Fiuza
INST SLAC National Accelerator Laboratory
HOURS 50 Million Core-Hours

Extreme-Scale Simulations for Multi-Wavelength Cosmology Investigations

PI Katrin Heitmann
INST Argonne National Laboratory
HOURS 125 Million Core-Hours
ALCF: 40M; OLCF: 10M; NERSC: 75M

Nuclear Spectra with Chiral Forces

PI Alessandro Lovato
INST Argonne National Laboratory
HOURS 35 Million Core-Hours

Nucleon Structure and Electric Dipole Moments with Physical Chirally Symmetric Quarks

PI Sergey Syritsyn
INST RIKEN BNL Research Center
HOURS 135 Million Core-Hours

ALCC 2018-2019

Chemistry

High-Fidelity Simulations of Flow and Heat Transfer During Motored Operation of an Internal Combustion Engine

PI Paul Fischer
INST Argonne National Laboratory
HOURS 30 Million Core-Hours

Computer Science

Portable Application Development for Next-Generation Supercomputer Architectures

PI T.P. Straatsma
INST Oak Ridge National Laboratory
HOURS 60 Million Core-Hours
ALCF: 30M; OLCF: 30M

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications

PI Robert Voigt
INST Leidos, Inc.
HOURS 199 Million Core-Hours
ALCF: 100M; OLCF: 79M; NERSC: 20M

Earth Science

Large-Eddy Simulation Component of the Mesoscale Convective System Climate Model Development and Validation (CMDV-MCS) Project

PI William Gustafson
INST Pacific Northwest National Laboratory
HOURS 54 Million Core-Hours

Investigating the Impact of Improved Southern Ocean Processes in Antarctic-Focused Global Climate Simulations

PI Mark Petersen
INST Los Alamos National Laboratory
HOURS 105 Million Core-Hours
ALCF: 35M; OLCF: 5M; NERSC: 65M

Energy Technologies

Multiphase Flow Simulations of Nuclear Reactor Flows

PI Igor Bolotnov
INST North Carolina State University
HOURS 130 Million Core-Hours

High-Fidelity Simulation for Molten Salt Reactors: Enabling Innovation Through Petascale Computing

PI Elia Merzari
INST Argonne National Laboratory
HOURS 140 Million Core-Hours

HPC4EnergyInnovation ALCC End-Station

PI Peter Nugent
INST Lawrence Berkeley National Laboratory
HOURS 170 Million Core-Hours
ALCF: 20M; OLCF: 100M; NERSC: 50M

High-Fidelity Numerical Simulation of Wire-Wrapped Fuel Assemblies: Year 2

PI Aleksandr Obabko
INST Argonne National Laboratory
HOURS 84 Million Core-Hours

Engineering

Analysis and Mitigation of Dynamic Stall in Energy Machines

PI Anupam Sharma
INST Iowa State University
HOURS 52 Million Core-Hours

Materials Science

Large-Scale Simulations of Heterogeneous Materials for Energy Conversion Applications

PI Giulia Galli
INST The University of Chicago
Argonne National Laboratory
HOURS 100 Million Core-Hours

Imaging and Controlling Elemental Contrast of Nanocluster in Intense X-Ray Pulses

PI Phay Ho
INST Argonne National Laboratory
HOURS 90 Million Core-Hours

Impact of Grain Boundary Defects on Hybrid Perovskite Solar Absorbers

PI Wissam Saidi
INST University of Pittsburgh
HOURS 20 Million Core-Hours

Predictive Modeling and Machine Learning for Functional Nanoporous Materials

PI J. Ilja Siepmann
INST University of Minnesota
HOURS 58 Million Core-Hours
ALCF: 42M; NERSC: 16M

Modeling Fusion Plasma Facing Components

PI Brian Wirth
INST Oak Ridge National Laboratory
University of Tennessee
HOURS 165 Million Core-Hours
ALCF: 80M; OLCF: 60M; NERSC: 25M

Physics

Hadronic Light-by-Light Scattering and Vacuum Polarization Contributions to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions

PI Thomas Blum
INST University of Connecticut
HOURS 162 Million Core-Hours

Emulating the Universe

PI Katrin Heitmann
INST Argonne National Laboratory
HOURS 50 Million Core-Hours
ALCF: 10M; OLCF: 40M

Scaling LHC Proton-Proton Collision Simulations in the ATLAS Detector

PI Eric Lancon
INST Brookhaven National Laboratory
HOURS 160 Million Core-Hours
ALCF: 80M; OLCF: 80M

Nucleon Structure and Electric Dipole Moments with Physical Chiral-Symmetric Quarks

PI Sergey Syritsyn
INST RIKEN BNL Research Center
HOURS 50 Million Core-Hours

Simulations of Laser Experiments to Study MHD Turbulence and Non-Thermal Charged Particles

PI Petros Tzeferacos
INST The University of Chicago
HOURS 22 Million Core-Hours

Semileptonic B- and D-meson Form Factors with High Precision

PI Ruth Van de Water
INST Fermi National Accelerator Laboratory
HOURS 247 Million Core-Hours

ALCF Data Science Program

Massive Hyperparameter Searches on Deep Neural Networks Using Leadership Systems

PI Pierre Baldi
INST University of California, Irvine

Enabling Multiscale Physics for Industrial Design Using Deep Learning Networks

PI Rathakrishnan Bhaskaran
INST GE Global Research

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

PI Taylor Childers
INST Argonne National Laboratory

Data-Driven Molecular Engineering of Solar-Powered Windows

PI Jacqueline Cole
INST University of Cambridge

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

PI Fabien Delalondre
INST Ecole Federale Polytechnique de Lausanne

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

PI Doga Gursoy
INST Argonne National Laboratory

Realistic Simulations of the LSST Survey at Scale

PI Katrin Heitmann
INST Argonne National Laboratory

Constructing and Navigating Polymorphic Landscapes of Molecular Crystals

PI Alexandre Tkatchenko
INST University of Luxembourg

Aurora Early Science Program

Extending Moore's Law Computing with Quantum Monte Carlo

PI Anouar Benali
INST Argonne National Laboratory

Exascale Computational Catalysis

PI David Bross
INST Argonne National Laboratory

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang
INST Princeton Plasma Physics Laboratory

Machine Learning for Lattice Quantum Chromodynamics

PI William Detmold
INST Massachusetts Institute of Technology

NWChemEx: Tackling Chemical, Materials, and Biochemical Challenges in the Exascale Era

PI Thom Dunning
INST Pacific Northwest National Laboratory

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI Nicola Ferrier
INST Argonne National Laboratory

Dark Sky Mining

PI Salman Habib
INST Argonne National Laboratory

Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann
INST Argonne National Laboratory

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI Kenneth Jansen
INST University of Colorado Boulder

Extreme-Scale Unstructured Adaptive CFD

PI Kenneth Jansen
INST University of Colorado Boulder

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials

PI Noa Marom
INST Carnegie Mellon University

Simulating and Learning in the ATLAS Detector at the Exascale

PI James Proudfoot
INST Argonne National Laboratory

Extreme-Scale In-Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations

PI Amanda Randles
INST Duke University
Oak Ridge National Laboratory

Virtual Drug Response Prediction

PI Rick Stevens
INST Argonne National Laboratory

Accelerated Deep Learning Discovery in Fusion Energy Science

PI William Tang
INST Princeton Plasma Physics Laboratory

2018 Director's Discretionary

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

Biological Sciences

Computational Analysis of Brain Connectomes for Alzheimer's Disease

PI Jiook Cha
INST Columbia University
HOURS 10 Million Core-Hours

Developmental Trajectory of Brain and Cognition in Youth in Physiological and Pathological Conditions

PI Jiook Cha
INST Columbia University
HOURS 10 Million Core-Hours

Cancer Workflow Toolkit

PI Justin Wozniak
INST Argonne National Laboratory
HOURS 6 Million Core-Hours

Chemistry

Improving Gas Reactor Design with Complex Non-Standard Reaction Mechanisms in a Reactive Flow Model

PI Marc Day
INST Lawrence Berkeley National Laboratory
HOURS 5 Million Core-Hours

First-Principles Discovery of Design Rules for Anion Exchange Membranes with High Hydroxide Conductivity

PI Mark Tuckerman
INST New York University
HOURS 7 Million Core-Hours

Computer Science

System Software to Enable Data-Intensive Science

PI Philip Carns
INST Argonne National Laboratory
HOURS 4 Million Core-Hours

MPICH - A High-Performance and Widely Portable MPI Implementation

PI Ken Raffenetti
INST Argonne National Laboratory
HOURS 10 Million Core-Hours

Earth Science

Simulating Global Terrestrial Carbon Sequestration and Carbon Transport to Aquatic Ecosystems

PI Jinxun Lin
INST United States Geological Survey
HOURS 3 Million Core-Hours

Engineering

Simulation of Supersonic Combustion

PI Farzad Mashayek
INST University of Illinois at Chicago
HOURS 4 Million Core-Hours

High-Fidelity Simulation of Supersonic Turbulent Flow-Structure Interaction and Mixing

PI Ivan Bermejo-Moreno
INST University of Southern California
HOURS 6 Million Core-Hours

Data Analysis of Turbulent Channel Flow at High Reynolds Number

PI Robert Moser
INST University of Texas at Austin
HOURS 6 Million Core-Hours

Scalability of Grid-to-Grid Interpolation Algorithms for Internal Combustion Engine Simulations

PI Saumil Patel
INST Argonne National Laboratory
HOURS 8 Million Core-Hours

Computation of Transitional and Turbulent Drop Flows for Liquid Carbon Dioxide Drops Rising in Seawater

PI Arne J. Pearlstein
INST University of Illinois at Urbana-Champaign
HOURS 4 Million Core-Hours

HPC4Mfg: Modeling Paint Behavior During Rotary Bell Atomization

PI Robert Saye
INST Lawrence Berkeley National Laboratory
HOURS 8 Million Core-Hours

Full Core PWR Simulation Using 3D Method of Characteristics

PI Kord Smith
INST Massachusetts Institute of Technology
HOURS 12 Million Core-Hours

Materials Science

Quantum Monte Carlo Study of Spin-Crossover Transition in Fe(II)-Based Complexes

PI Hanning Chen
INST George Washington University
HOURS 7 Million Core-Hours

Rational Design of Ultrastrong Composites

PI Hendrik Heinz
INST University of Colorado Boulder
HOURS 3 Million Core-Hours

Phase Transitions in Water-Ice-Vapor System

PI Subramanian Sankaranarayanan
INST Argonne National Laboratory
HOURS 64 Million Core-Hours

Large-Scale Atomistic Simulations for Predicting Nano/Microstructures and Properties in Solidification of Metals

PI Asle Zaeem
INST Missouri University of Science and Technology
HOURS 4 Million Core-Hours

2T-MD Model Simulations of High Energy Ion Irradiation

PI Eva Zarkadoula
INST Oak Ridge National Laboratory
HOURS 2 Million Core-Hours

Physics

Scalable Reconstruction of X-Ray Scattering Imaging for Nanomaterials

PI Wei Jiang
INST Argonne National Laboratory
HOURS 6 Million Core-Hours

Hadronic Light-by-Light Scattering and Vacuum Polarization Contributions to the Muon g-2 from LQCD - Finite-Volume Studies

PI Christoph Lehner
INST Brookhaven National Laboratory
HOURS 20 Million Core-Hours

MARS Energy Deposition and Neutrino Flux Simulations

PI Nikolai Mokhov
INST Fermilab
HOURS 18 Million Core-Hours

Scaling and Performance Enhancement of an Astrophysical Plasma Code

PI Brian O'Shea
INST Michigan State University
HOURS 1 Million Core-Hours

Particle-in-Cell Simulations of Explosive Reconnection in Relativistic Magnetically Dominated Plasmas

PI Lorenzo Sironi
INST Columbia University
HOURS 2 Million Core-Hours

Simulations of Laser Experiments to Study the Origin of Cosmic Magnetic Fields

PI Petros Tzeferacos
INST The University of Chicago
HOURS 5 Million Core-Hours

Quantum Monte Carlo Modeling of Strongly Correlated Electronic Systems

PI Huihuo Zheng
INST Argonne National Laboratory
HOURS 3 Million Core-Hours

About the Argonne Leadership Computing Facility

Argonne's Leadership Computing Facility Division operates the Argonne Leadership Computing Facility (ALCF) 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

Argonne is a U.S. Department of Energy Laboratory managed by UChicago Argonne, LLC, under contract DE-AC02-06CH11357. The Laboratory's main facility is outside of Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, visit www.anl.gov.

Availability of this Report (ANL/ALCF-18/3)

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

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

U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd.
Alexandra, VA 22312

phone | 800.553.NTIS (6847) or 703.605.6000
fax | 703.605.6900
orders@ntis.gov
www.ntis.gov

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

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

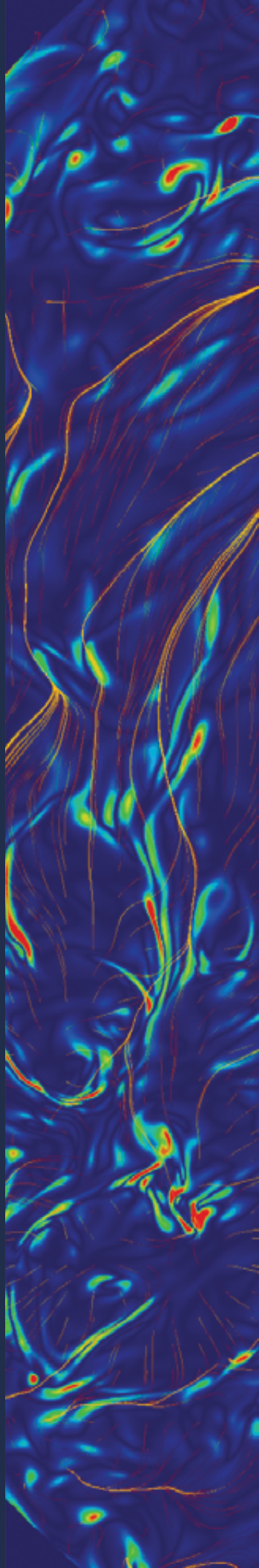
phone | 865.576.8401
fax | 865.576.5728
reports@adonis.osti.gov
www.osti.gov

Editorial Team: Beth Cerny, Jim Collins, Nils Heinonen, Madeleine O'Keefe, John Spizzirri, and Laura Wolf

Design and production: Sandbox Studio, Chicago

Argonne NATIONAL LABORATORY

CONTACT
ALCF Communications
media@alcf.anl.gov
alcf.anl.gov



U.S. DEPARTMENT OF ENERGY

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