Argonne Leadership Computing Facility

2018 Annual Report

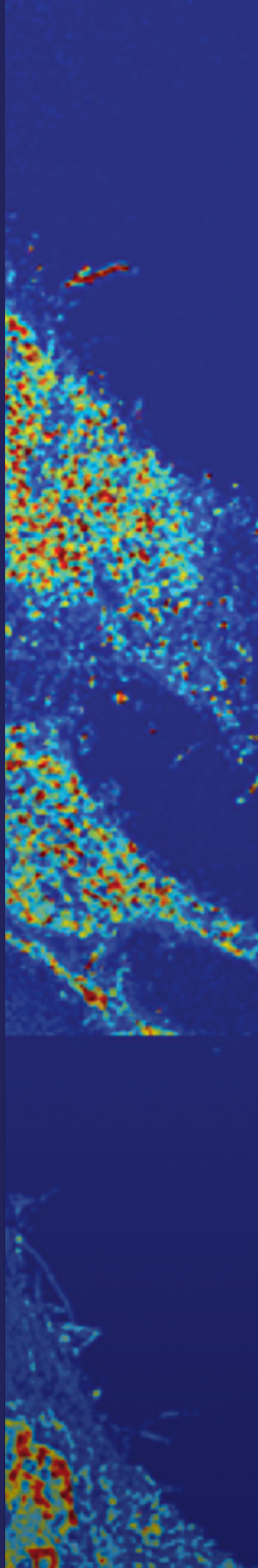
A visualization of the turbulent envelope of a luminous blue variable star surrounding the central high-density core. These massive, evolved stars display large variations in their luminosity. Using the ALCF's Mira supercomputer, a team led by researchers from the University of California, Santa Barbara, found that helium opacity plays an important part in triggering the outbursts and in setting their effective temperature of around 9,000 Kelvin. The team predicts that these stars should also show variability at the 10–30 percent level on a timescale of days. Their findings were published in the journal Nature and also featured on the cover (doi: 10.1038/s41586-018-0525-0). Computing time for this work was awarded through the U.S. Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. *Image: Joseph A. Insley, Argonne National Laboratory; Matteo Cantiello, Flatiron Institute; James Stone, Princeton University; Eliot Quataert, University of California, Berkeley; Lars Bildsten, Omer Blaes, and Yan-Fei Jiang, University of California, Santa Barbara*

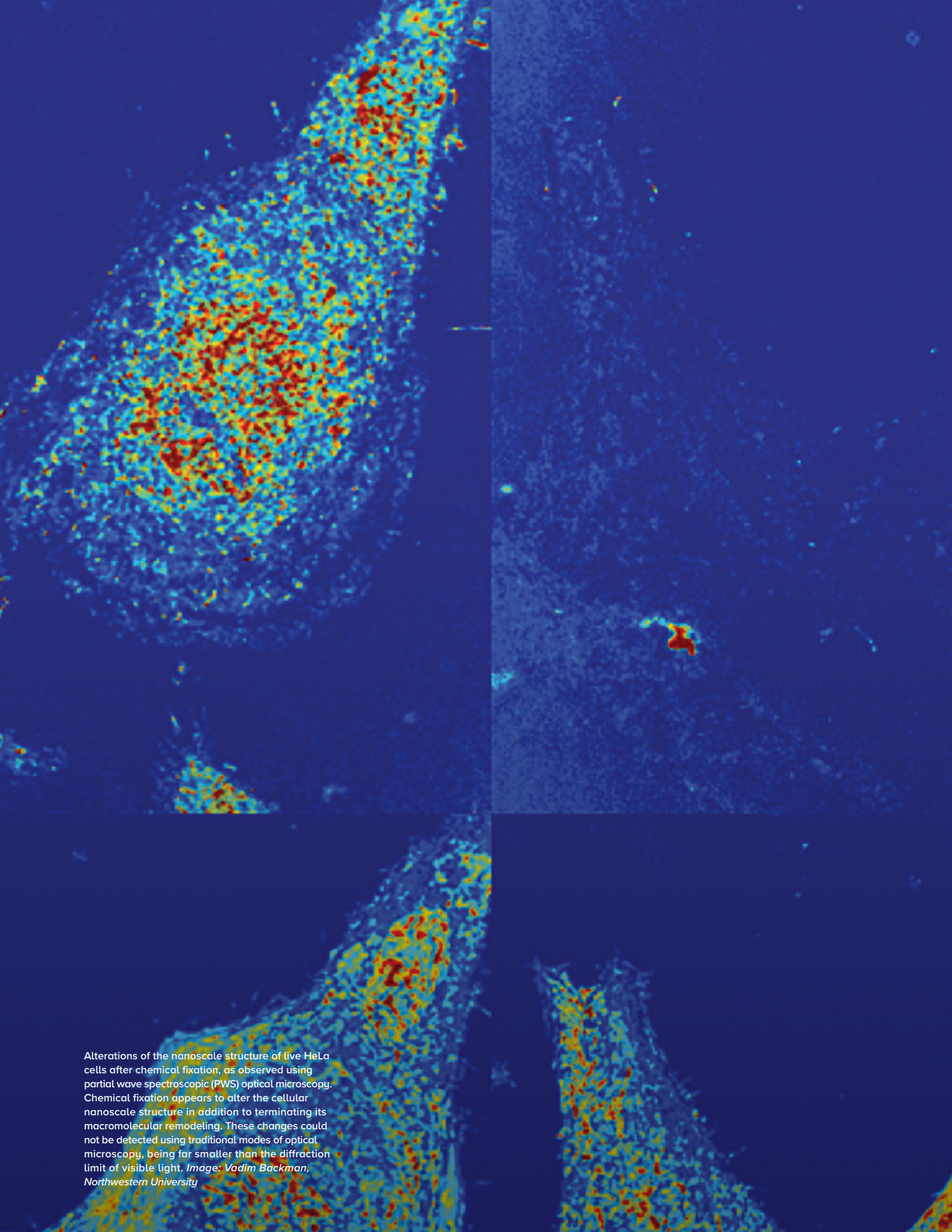
CONTENTS

2018 Annual Report

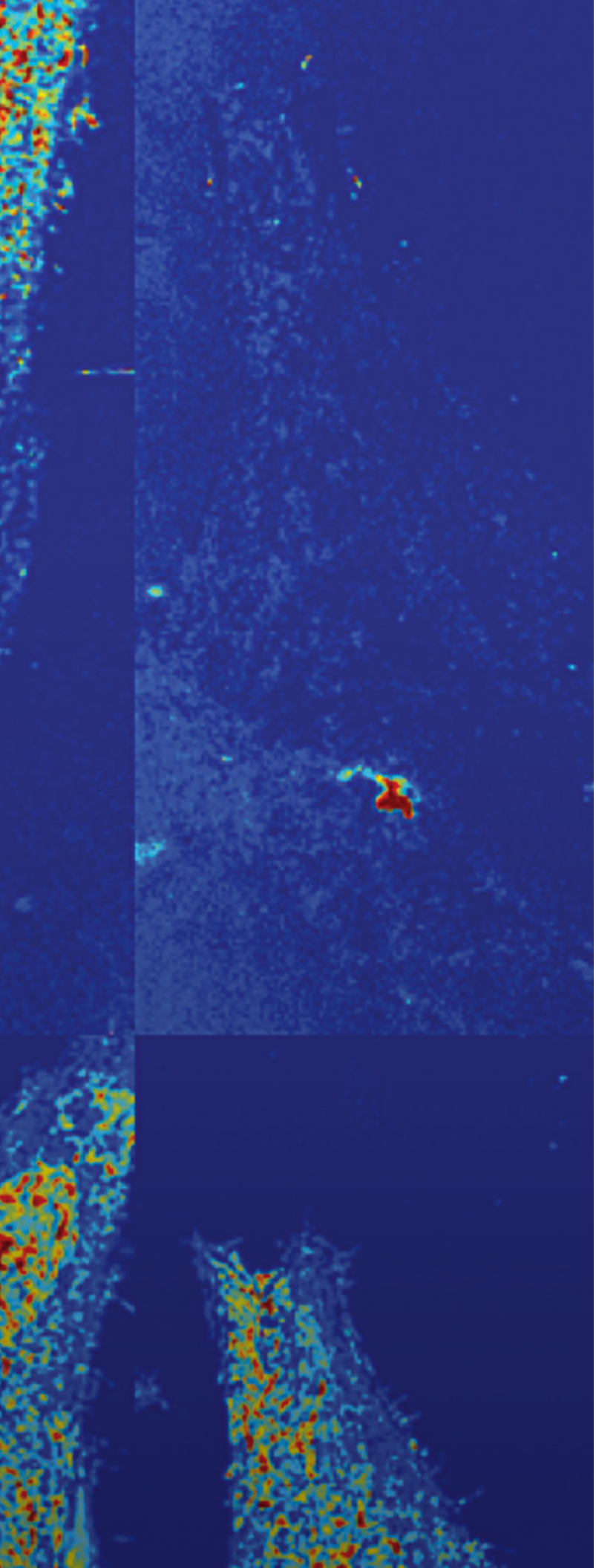
YEAR IN REVIEW

The Argonne Leadership Computing Facility enables breakthroughs in science and engineering by providing supercomputing resources and expertise to the research community.





Alterations of the nanoscale structure of live HeLa cells after chemical fixation, as observed using partial wave spectroscopic (PWS) optical microscopy. Chemical fixation appears to alter the cellular nanoscale structure in addition to terminating its macromolecular remodeling. These changes could not be detected using traditional modes of optical microscopy, being far smaller than the diffraction limit of visible light. *Image: Vadim Backman, Northwestern University*



ALCF Leadership

MICHAEL E. PAPKA
ALCF Director

High-performance computing is a principal research tool in a growing number of scientific domains. As a leadership computing facility dedicated to open science, the ALCF is actively working to broaden the impact of its supercomputers by making HPC more approachable to more users.

In 2018, we continued to build up programs and efforts that reinforce our overall simulation, learning, and data analysis capabilities as a facility. We also enhanced our services to better meet our users' needs and workflow preferences.

The Aurora Early Science Program added 10 data science and machine learning projects to support the ALCF's new paradigm for scientific computing, which expands on traditional simulation-based research to include data science and machine learning approaches. Aurora is the ALCF's future exascale computer, and this program is designed to prepare key applications, libraries, and infrastructure for the architecture and scale of the system. These projects will be laying the path for hundreds of future users while delivering actual science.

The ALCF Data Science Program also added a new set of forward-looking projects that will utilize machine learning, deep learning, and other artificial intelligence methods to enable data-driven discoveries. The targets of these projects range from the analysis of astrophysical events to the discovery of new material properties to innovative developments in x-ray imaging techniques.

The ALCF's evolving role in shaping how production science applications will move to emerging machine architectures is part of what makes the ALCF an especially attractive place to do research. Another part is being responsive to the HPC community's diversification and the practices and behaviors that our users engage in to do their work.

To that end, we have deployed Petrel, Jupyter, and Balsam—services and frameworks that help eliminate barriers to productivity and improve collaboration across scientific communities. We also deployed the Singularity container technology to allow users to easily migrate their software stack between resources and run the version of software that best meets their specific needs. Additionally, within the context of the nation's Exascale Computing Project, the ALCF is working on a Continuous Integration solution for HPC environments to better support ECP and existing user community computing needs.

This report is a great opportunity to highlight the year's activities and research at the ALCF, and also to recognize our amazing staff. Our highly talented teams keep our operations safe, our resources productive, and our users innovating. These are the people who essentially keep the science flowing, and I am grateful for the fine work they do every day.

JINI RAMPRAKASH
ALCF Deputy Director

MARK FAHEY
ALCF Director of Operations

This has been an eventful year for the ALCF as we continued to enable science with our two leadership-class machines while making progress on our efforts to design and deploy our next-generation system, Aurora. Our talented staff's skills and expertise are crucial to balancing the current needs of our users with the development of the new computing capabilities they will need in the future.

In 2018, the ALCF and our collaborators from DOE's Exascale Computing Project worked together to advance the nation's exascale goals through many mutually beneficial projects. Our collaborations include developing a Continuous Integration framework, exploring how containers can be used in the context of exascale resources, and offering joint HPC training events.

As the lead for our annual Operational Assessment Report, I have the pleasure of collecting our facility's most notable accomplishments, both scientific and technical, over the course of the year. The report provides an outlet for us to highlight stories of how our staff assists and educates users via workshops, webinars, and other training events; how we are installing new services and frameworks to advance scientific computing in this fast-changing technology landscape; and how we are growing our community through pipeline-building activities and outreach.

To improve the overall user experience at the ALCF, we actively solicit feedback from our users. The six members of our User Advisory Council provide advice and assistance to ALCF leadership on topics that impact the larger ALCF user community. And through the ALCF's annual user survey, we receive candid feedback from our users that helps to focus our efforts on providing the best possible experience for the researchers who leverage our computing resources to accelerate science.

With Theta and Mira, we continued to operate two production petascale systems for the research community. Both computing resources posted strong performance statistics, exceeding key DOE metrics for availability and utilization, while allowing our users to carry out large-scale computational studies.

In 2018, we made several enhancements to the ALCF computing environment. Our staff deployed a Continuous Integration (CI) solution using an open-source Jenkins automation server, providing users with a tool that can accelerate efforts to build, test, and optimize their codes for ALCF systems. We are working with DOE's Exascale Computing Project to set up a separate solution based on GitLab with the intention of providing seamless CI abilities across DOE laboratories. We significantly upgraded our tape archive infrastructure with the deployment of LT08 tape technology, which offers five times the capacity (12 TB) and more than double the transfer rate (360 MB/s) of our previous tape drives. In the business intelligence space, we launched new web-based reporting capabilities that provide up-to-date system data and metrics for both users and staff members.

In addition, we continued work to develop our improved user management system. The enhanced system, which will provide a number of new features for ALCF account and project management, is currently in beta testing and is set to be deployed in 2019. Next year, we also look forward to upgrading our storage and networking capabilities with the installation of a new Storage Area Network infrastructure and a new Global File System.

KATHERINE RILEY
ALCF Director of Science

KALYAN KUMARAN
ALCF Director of Technology

As we prepare for our future exascale system, Aurora, we have continued our efforts to advance the convergence of simulation, data science, and machine learning methods to drive discoveries and innovations on the supercomputers of today and tomorrow.

To support this paradigm shift, we are working to ensure that our facility's growth is aligned with the goals and needs of the larger research community. The ALCF Data Science Program continues to provide researchers with a mechanism to explore the use of advanced computational methods to enable data-driven discoveries, while our Aurora Early Science Program and DOE's INCITE program have expanded in scope to support data and learning projects alongside traditional simulation-based research. Partnering with the project teams supported by these allocation programs allows us to take a collaborative approach to exploring how to best utilize emerging methods and technologies at an unprecedented scale to accelerate science. In addition, we remain committed to providing training opportunities to educate our users about the tools, systems, and frameworks that are available to them. As part of this year's many offerings, we hosted two workshops focused on simulation, data, and learning topics to help our users improve their code performance and productivity on our systems.

Ultimately, we are here to enable science. And our user community produced some amazing results this past year using a variety of simulation, data, and learning techniques on our leadership-class machines. Their research resulted in more than 200 publications, including papers in high-impact journals such as *Science*, *Nature*, and *Physical Review Letters*. We can't wait to see what's in store for 2019.

We had a very productive year in not only supporting the ALCF's current production resources, but also contributing to various exascale projects, including the development of Aurora, several activities within DOE's Exascale Computing Project, and the CORAL-2 collaboration (the joint effort to procure DOE's next-generation supercomputers). Our group has grown significantly over the past year, adding several new staff members to focus on these important endeavors.

In 2018, we continued to enhance the ALCF computing environment by adding various tools and technologies for our user community. In the data science area, we deployed and optimized a diverse set of deep learning and machine learning software tools and frameworks on Theta. We also developed and deployed the Balsam service to enable scalable workflow management for production science. In addition, we remain actively engaged in compiler development, with staff members prototyping several new features that will be implemented to improve the usability of the Clang/LLVM compiler.

To help our users gain insights into large-scale datasets, we worked closely with project teams to help them visualize and analyze their data. One noteworthy example was a collaboration with an INCITE team investigating outbursts of luminous blue variable stars, which resulted in an impressive visualization that was featured on the cover of *Nature*.

All in all, our staff has helped the facility and the nation make great strides toward reaching exascale in 2021, while ensuring our users achieve optimal performance on Mira and Theta. Along the way, the team's work resulted in more than a dozen publications—including papers on MPI usage and performance, system architecture and deployment, and application development—and an R&D 100 Award for the development of Darshan, an HPC I/O characterization tool.

ALCF at a Glance

The Argonne Leadership Computing Facility (ALCF) is a U.S. Department of Energy (DOE) Office of Science User Facility that enables breakthroughs in science and engineering by providing supercomputing resources and expertise to the research community.

ALCF computing resources—available to researchers from academia, industry, and government agencies—support large-scale computing projects aimed at solving some of the world's most complex and challenging scientific problems. Through awards of supercomputing time and support services, the ALCF enables its users to accelerate the pace of discovery and innovation across disciplines.

Supported by the DOE's Advanced Scientific Computing Research (ASCR) program, the ALCF and its partner organization, the Oak Ridge Leadership Computing Facility, operate leadership-class supercomputers that are orders of magnitude more powerful than the systems typically used for open scientific research.

Core-hours of compute time

8.7B

Active projects*

410

Facility users*

954

Publications

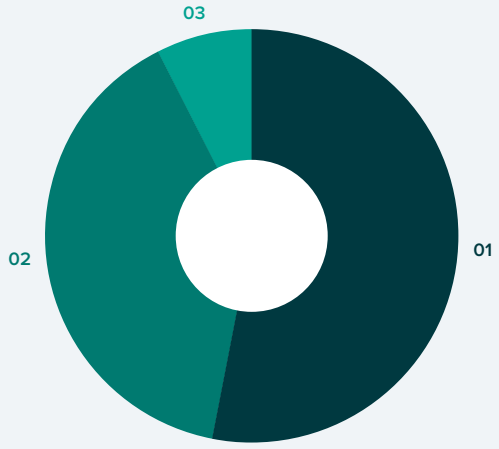
276

Supercomputers on the Top500 list

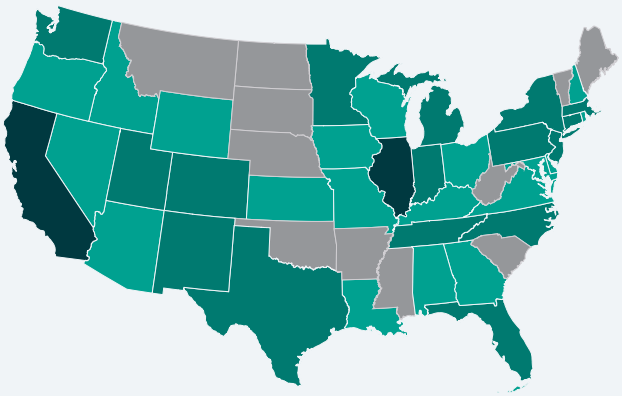
3

**Fiscal year 2018*

2018 ALCF Users by Affilliation



2018 U.S. ALCF Users by State



01 Academia

507

02 Government

376

03 Industry

71

100+ Users

California
Illinois

11–100 Users

Colorado
Iowa
Massachusetts
Michigan
North Carolina
New Jersey
New Mexico
New York
Oregon
Tennessee
Texas
Utah
Washington

01–10 Users

Alabama
Arizona
Connecticut
Washington D.C.
Delaware
Florida
Georgia
Hawaii
Indiana
Idaho
Kansas
Kentucky
Louisiana
Maryland
Minnesota
Missouri
New Hampshire
Nevada
Ohio
Pennsylvania
Rhode Island
Virginia
Wisconsin
Wyoming

PREPARING FOR EXASCALE

As a key player in the nation's efforts to deliver future exascale systems, the ALCF is helping to ensure researchers are ready for the next generation of leadership computing resources.

The ALCF's Exascale Future

As the future home to one of the world's first exascale systems, Aurora, the ALCF is making preparations for the next generation of scientific computing.

With Aurora scheduled to arrive in 2021, the ALCF has been actively engaged in several activities designed to enable dramatic scientific advances on its next-generation system.

From managing the Aurora Early Science Program and expanding the facility's data center to supporting research involving emerging data science and machine learning techniques, the ALCF will be ready to hit the ground running when its Intel-Cray exascale system becomes available to the research community.

The most visible evidence of Aurora's impending arrival is the construction taking place at the Theory and Computing Sciences (TCS) Building at Argonne National Laboratory.

The TCS Building is adding 15,000 square feet of data center space that Argonne will lease to house its future systems. The building's utilities are also being upgraded to increase the power and cooling services provided to ALCF supercomputers. This work includes the installation of an additional 60MW feed to the building and an upgrade to the laboratory's chilled water plant to provide an additional 17,000 tons of cooling to accommodate up to 60MW of heat rejection.

A NEW MODEL FOR SCIENTIFIC COMPUTING

To take full advantage of exascale computing power, the ALCF continues to help define a paradigm for scientific computing predicated on the convergence of simulation, data science, and machine learning. This effort will reframe the way its next-generation computing resources are used to enable discoveries and innovation.

While simulation has long been the cornerstone of scientific computing, the ALCF has been working to create an environment that also supports data science and machine learning-based research 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 can better enable data-driven discoveries across 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.

In addition, Argonne recently created 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 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.

The Theory and Computing Sciences Building at Argonne National Laboratory is adding 15,000 square feet of data center space to house the ALCF's future systems.

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

Secretary of Energy Rick Perry (second from right) toured the Argonne Leadership Computing Facility with Rick Stevens, Associate Laboratory Director for Argonne's Computing, Environment and Life Sciences Directorate (third from left). Accompanying the Secretary were Argonne Director Paul Kearns, U.S. Representative Bill Foster, DOE's Joanna Livengood, and others.

ADVANCING SCIENCE WITH DATA-CENTRIC TOOLS AND SERVICES

Data has always been an integral part of leadership-scale computing, but the ever-growing amount of data being produced by 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 capabilities made possible by its leadership computing resources, allowing users to undertake large-scale science campaigns involving petabytes of data.

By providing facility users with high-performing, scalable machine learning software, analytics frameworks, data management services, workflow packages, and runtime optimizations, the ALCF's goal is to drive advances in scientific machine learning and the analysis of big data.

For example, the ALCF is collaborating with Globus to provide Petrel, a data management and sharing platform designed to connect experimental data sources to ALCF computing resources. Petrel makes it easy to store and manage massive datasets, leverage ALCF systems for data exploration and analysis, and share data with external collaborators. Multiple Argonne teams are benefitting from Petrel's data management capabilities, including scientists from the Advanced Photon Source using the platform to enable the analysis and sharing of experimental data; a neuroscience project storing large-scale datasets from electronic microscopy experiments aimed at mapping the brain; and a computational cosmology team storing and sharing datasets produced by their simulations with the HACC code.

The ALCF also deployed a Continuous Integration, or CI, service that uses an open-source Jenkins automation server to provide researchers with a tool for improving the robustness of their code at the ALCF. The Jenkins-based CI tool helps users eliminate build and deployment issues, which in turn improves development cycles; provides a timely feedback loop with developers; and results in higher quality deliverables with reduced development time.

Other new services and tools now available to ALCF users include Balsam, an ALCF-developed workflow management service that helps automate and simplify the task of running large-scale job campaigns on supercomputers; Singularity, an open-source framework for creating and running containers on HPC systems; and a variety of scalable frameworks for machine learning and deep learning (e.g., TensorFlow, Keras, PyTorch, Scikit-Learn, Horovod, and Cray ML).

The ALCF's evolving suite of tools and services is part of a continuing effort to provide resources that enable scientific discoveries on current and future systems, help to eliminate barriers to productively using the facility's systems, enhance collaboration among research teams, and integrate with user workflows to produce seamless, usable environments.

TRAINING USERS ON EMERGING HPC TOOLS AND TECHNIQUES

The ALCF expanded its training programs in 2018 with new offerings intended to educate researchers on nascent HPC tools and technologies.

The facility hosted two Simulation, Data, and Learning workshops to connect users with ALCF staff members and experts from Intel, Cray, and Arm to provide guidance on using systems, tools, frameworks, and techniques that can help their advance research. The hands-on workshops were designed to teach attendees how such resources can be used to improve productivity, while elucidating potential research directions that may not have been possible in the past.

The annual Argonne Training Program on Extreme-Scale Computing is designed to educate researchers on the tools and techniques needed to carry out scientific computing research on the world's most powerful supercomputers.

The Aurora Early Science Program (ESP) kicked off a training series designed to prepare ESP teams for the facility's future exascale system. The web-based series offers tutorials on topics and tools relevant to leadership-scale computing resources, with an emphasis on data-intensive and machine learning subjects.

The ALCF continued its monthly Developer Sessions to foster discussion between the developers of emerging hardware and software and the early users of the technologies. Speakers in this webinar series have included developers from the ALCF, Intel, and Cray, covering topics such as performance profiling tools, TensorFlow, and the Global Extensible Open Power Manager (GEOPM).

ALCF staff members also continue to organize and manage the annual Argonne Training Program on Extreme-Scale Computing (ATPESC), which is funded by DOE's Exascale Computing Project. ATPESC is an intensive, two-week program that teaches attendees to the key skills, approaches, and tools needed to design, implement, and execute computational science and engineering applications on current supercomputers and the extreme-scale systems of the future.

ARGONNE TESTBEDS ENABLE PIONEERING COMPUTING RESEARCH

In addition to operating production supercomputers for science, the ALCF co-leads Argonne's Joint Laboratory for System Evaluation (JLSE). By providing access to leading-edge testbeds, the JLSE allows researchers to assess next-generation hardware and software platforms, develop capabilities that will improve science productivity on future systems, and collaborate with industry partners on prototype HPC technologies.

In 2018, JLSE resources supported 380 users participating in 60 research projects.

Certain efforts are specifically aimed at enabling science in the exascale era. For example, one research team is using JLSE resources to further the development of Argo, a new exascale operating system and runtime system designed to support extreme-scale scientific computation. Another team from the Center for Efficient Exascale Discretizations (CEED), a co-design center within DOE's Exascale Computing Project, is using the JLSE's diverse set of machines for portability development, scalable algorithm development, and performance testing.

A number of JLSE projects are exploring the potential of deep learning approaches. One such effort is using JLSE resources to automate the deep neural architecture search to build deep learning models for scientific datasets, while another research team is focused on identifying ways in which deep learning can be used to improve lossy compression of scientific data from simulations and experimental instruments.

Quantum computing is another popular area of research at the JLSE, with users leveraging the laboratory's Atos Quantum Learning Machine to study the simulation of quantum sensing techniques and the use of quantum algorithms for simulating fermion systems.

PARTNERING WITH DOE'S EXASCALE COMPUTING PROJECT

Beyond its preparations for the arrival of Aurora, Argonne is also a key contributor to the DOE's Exascale Computing Project (ECP), a multi-lab initiative to accelerate the delivery of a capable exascale computing ecosystem.

Launched in 2016, the ECP's mission is to build an ecosystem that encompasses applications, system software, hardware technologies, architectures, and workforce development to pave the way for the deployment of the nation's first exascale systems.

Simulation
Data
Learning

The ALCF is advancing scientific computing through a convergence of simulation, data science, and machine learning methods.

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 has a strong presence on the ECP leadership team, with Andrew Siegel serving as the Director of Application Development, Susan Coghlan serving as Deputy Director of Hardware and Integration, and David Martin serving as Co-Executive Director of the ECP Industry Council. Several Argonne researchers are also engaged in ECP projects and working groups focused on application development, software development, and hardware technology. For example, ALCF staff members are participating in a multi-lab effort to develop a GitLab-based solution that will provide seamless Continuous Integration capabilities across DOE's computing facilities to aid exascale code development efforts.

In February, many of the Argonne contributors attended the ECP Annual Meeting to engage in technical conversations, project discussions, and facility-specific breakouts. ALCF researchers participated in several planning meetings with ECP and the other DOE computing facilities at OLCF and NERSC to develop and deploy the ECP/Facilities engagement plan. Facility staff also worked with the ECP training lead to promote ECP training activities to the ALCF user community.

In addition to the staff contributions, Argonne computing resources are playing a role in helping the ECP achieve its goals, with several ECP research teams tapping Theta and JLSE systems for development work.

Together, all of these efforts are preparing the research community to harness the immense computing power of Aurora and other future exascale systems to drive a new era of scientific discoveries and technological innovations.

Readying Aurora for Science on Day One

Researchers participating in the Aurora Early Science Program are helping to optimize software applications and tools, and characterize the behavior of the ALCF's next-generation system.

The Aurora Early Science Program (ESP) is designed to prepare key applications for the architecture and scale of the exascale supercomputer, and field-test compilers and other software to pave the way for other production applications to run on the system.

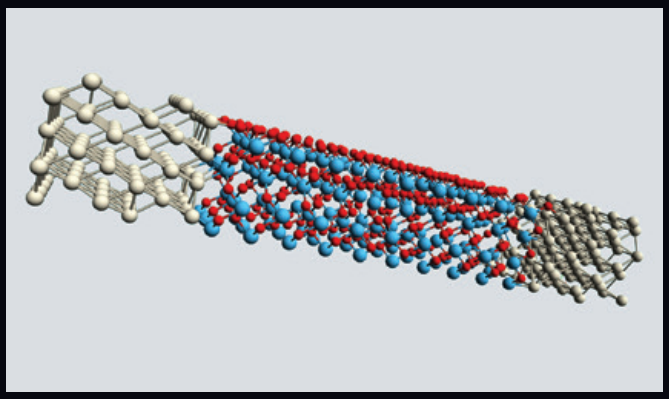
Through open calls for proposals, the ALCF program has awarded pre-production computing time and resources to five simulation projects, five data projects, and five learning projects.

Each ESP team is made up of application developers, domain science experts, and an ALCF postdoctoral appointee. In collaboration with experts from Intel and Cray, ALCF staff will help train the teams on the Aurora hardware design and how to program it.

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

Together, the projects will investigate a wide range of computational research areas critical to enabling science in the exascale era. This includes mapping and optimizing complex workflows, exploring new machine learning methodologies, stress-testing I/O hardware and other emerging technologies, and enabling connections to large-scale experimental data sources, such as CERN's Large Hadron Collider, for analysis and guidance.

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

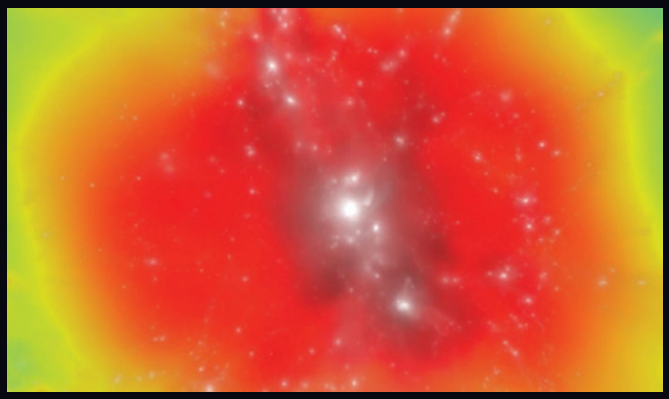
PI	Anouar Benali
INST	Argonne National Laboratory
SFTWR	QMCPACK, MKL, FFTW, BLAS/LAPACK, HDF5, ADIOS, libXML

SCIENCE

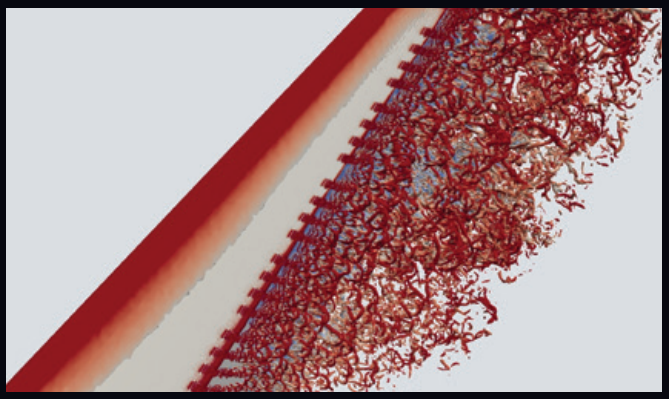
This project will carry out massive quantum Monte Carlo simulations to identify possible paths forward for extending silicon complementary metal-oxide-semiconductor (Si-CMOS)-based computing technologies beyond Moore's Law.

DEVELOPMENT

The development of QMCPACK focuses on enabling the code's kernel to run efficiently on the exascale system, while managing multi-level memory/storage hierarchy and exposing additional layers of parallelism. The team also worked on improving high-throughput internal tools to drive large campaign runs on Aurora.



This image shows the baryon density (white) and the baryon temperature (color) of a cluster of galaxies. *Image: JD Emberson and the HACC team, Argonne National Laboratory*



Flow over a vertical tail/rudder assembly (grey surface) with 24 active synthetic jets which introduce vortical structures (visualized by isosurfaces of vorticity colored by local flow speed) that alter the flow, reducing separation, improving rudder performance, and thereby allowing future aircraft designs to lower drag and fuel consumption. *Image: Jun Fang, Argonne National Laboratory*

Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann
INST Argonne National Laboratory
SFTWR HACC, Thrust

SCIENCE

Researchers will use Aurora to perform 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. These simulations will help guide and interpret observations from large-scale cosmological surveys.

DEVELOPMENT

The team will build upon the hydrodynamics capabilities of the HACC framework to enable the modeling of observations across multiple length scales and wavebands simultaneously at high fidelity. Preparing the project's large suite of analysis tools for Aurora will be a valuable portability exercise for future system users.

Extreme-Scale Unstructured Adaptive CFD

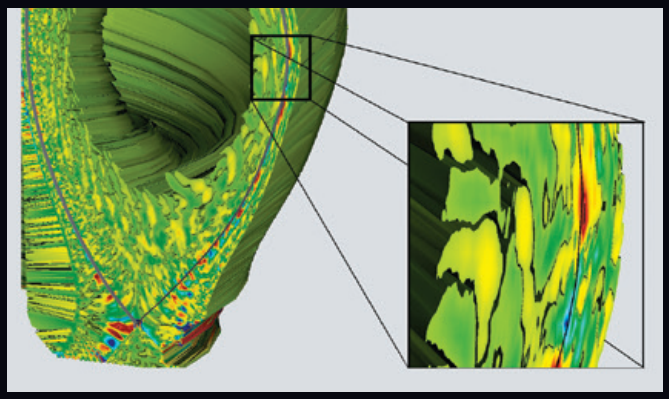
PI Kenneth Jansen
INST University of Colorado Boulder
SFTWR PHASTA, PETSc, PUMI, Zoltan, parMETIS

SCIENCE

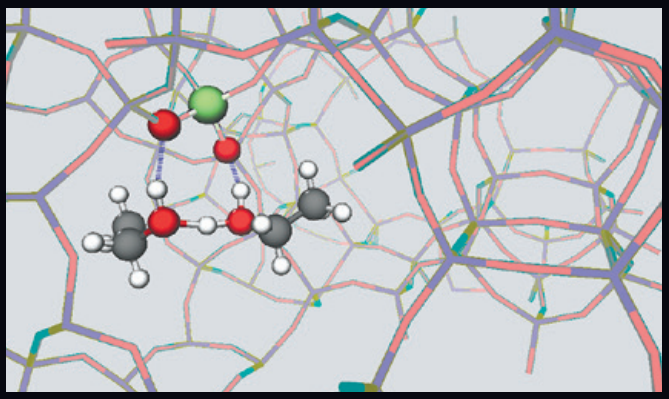
This project will perform simulations of unprecedented scale in two complex flow regimes: aerodynamic flow control and multiphase flow. The simulations will help inform the design of next-generation aircraft and nuclear reactors by providing insights into 3D active flow control at flight scale and reactor heat exchanger flow physics, respectively.

DEVELOPMENT

The strong scaling needs of PHASTA will help stress test and improve Aurora's advanced interconnect. PHASTA's I/O capabilities will be enhanced to take advantage of Aurora's I/O system. This project will also make use of PETSc, PUMI, and Zoltan, preparing these libraries for future use on Aurora.



Structure of density eddies from plasma turbulence in a typical present-day tokamak edge plasma. The transition from a connected core-like turbulence eddies to isolated turbulence across the magnetic separatrix surface (black line) can be seen. *Image: Dave Pugmire, Oak Ridge National Laboratory; Seung-Hoe Ku, Princeton Plasma Physics Laboratory*



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

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang
INST Princeton Plasma Physics Laboratory
SFTWR XGC, PETSc, PSPLINE, LAPACK, ADIOS, parMETIS

SCIENCE

By advancing the understanding and prediction of plasma confinement at the edge, the team's simulations on Aurora will help guide fusion experiments, such as ITER, and accelerate efforts to achieve fusion energy production.

DEVELOPMENT

XGC's problem size is expected to demand a significant fraction of the Aurora system. Computational and mathematical techniques will be developed to take advantage of Aurora's hardware structure efficiently, and to utilize memory structure for extreme-size restart data and heterogeneous physics data. This project also offers a potential comparison case for multilevel parallelization using MPI, OpenMP, and OpenACC, together with CUDA, on CPU-GPUs.

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

PI Thom H. Dunning, Jr.
INST University of Washington and Pacific Northwest National Laboratory
SFTWR NWChemEx

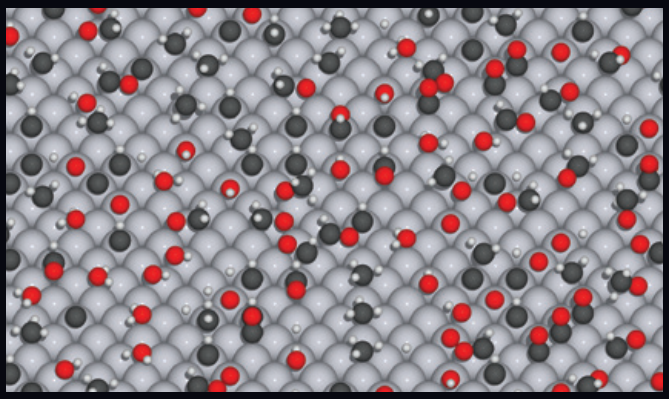
SCIENCE

This project will use NWChemEx to address two challenges related to the production of advanced biofuels: the development of stress-resistant biomass feedstock and the development of catalytic processes to convert biomass-derived materials into fuels.

DEVELOPMENT

The team is redesigning and reimplementing the NWChem code to enhance its scalability, performance, extensibility, and portability, positioning NWChemEx to serve as the framework for a community-wide effort to develop a comprehensive, next-generation molecular modeling package. The NWChemEx code will implement state-of-the-art algorithms for Hartree-Fock, density functional theory, and coupled cluster calculations. It will be able to effectively use multiple levels of memory as well as a partitioned global address space (PGAS) programming model to ensure that NWChemEx takes maximum advantage of the extraordinary computational capability of the Aurora exascale computing system.

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 Laboratories*

DATA

Exascale Computational Catalysis

PI	David Bross
INST	Argonne National Laboratory
SFTWR	NRRAO, RMG, PostgreSQL, Fitpy, KinBot, Sella, Balsam, NWChemEx

SCIENCE

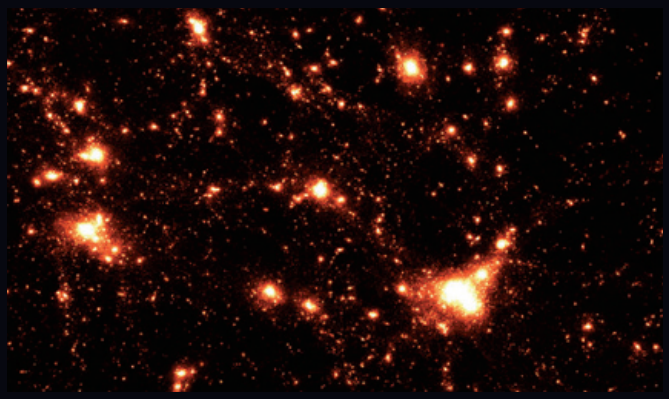
Researchers will develop software tools to facilitate and significantly speed up the quantitative description of crucial gas-phase and coupled heterogeneous catalyst/gas-phase chemical systems. Such tools promise to enable revolutionary advances in predictive catalysis, crucial to addressing DOE grand challenges including both energy storage and chemical transformations.

DEVELOPMENT

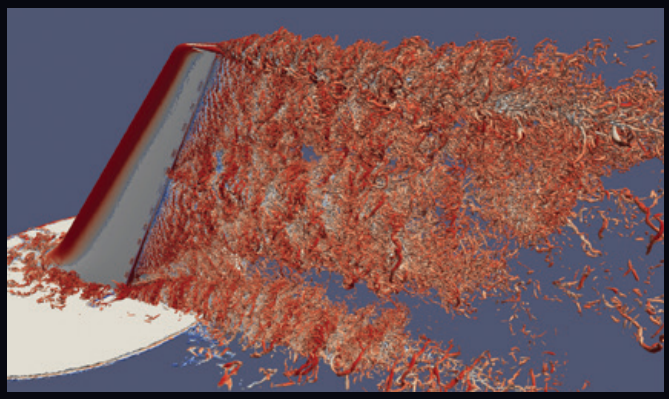
This project's diverse set of cheminformatics tools and databases will stress Aurora's deep learning software and hardware capabilities. The scientific workflow, which couples simulation, data, and learning methods, is expected to benefit from Aurora's advanced I/O hardware.

DATA/LEARNING METHODS

Regression, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, image and signal processing, databases, and graph analytics



HACC cosmology simulations allow researchers to track the evolution of structures in great detail. *Image: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory*



Flow visualization through an isosurface of instantaneous Q criterion colored by speed. *Image: Kenneth Jansen, University of Colorado Boulder*

Dark Sky Mining

PI	Salman Habib
INST	Argonne National Laboratory
SFTWR	Custom analyses, containers, TensorFlow, hyperparameter optimization, HACC, CosmoTools

SCIENCE

By implementing cutting-edge data-intensive and machine learning techniques, this project will usher in a new era of cosmological inference targeted for the Large Synoptic Survey Telescope (LSST).

DEVELOPMENT

Data mining and machine learning approaches, such as Gaussian process modeling, variational autoencoders, and Bayesian optimization, will stress the deep learning capabilities of Aurora's architecture and software. The project's end-to-end workflow is expected to benefit from the system's I/O hardware and access to databases.

DATA/LEARNING METHODS

Classification, regression, clustering, dimensionality reduction, advanced/parallel workflows, advanced statistics, reduced/surrogate models, image and signal processing, databases, deep learning, and graph analytics

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI	Kenneth Jansen
INST	University of Colorado Boulder
SFTWR	VTK, Paraview, PHASTA, PETSc

SCIENCE

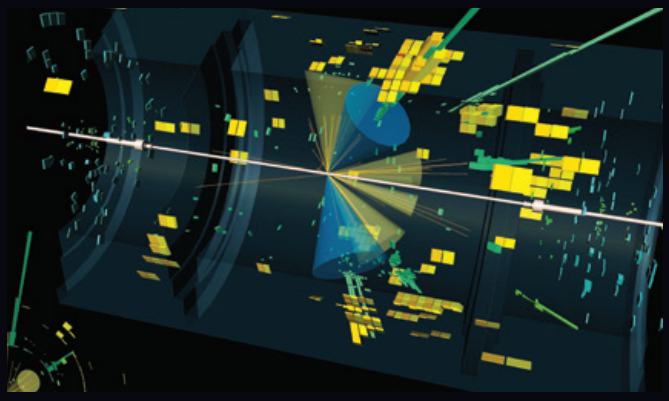
This project will develop data analytics and machine learning techniques to greatly enhance the value of flow simulations, culminating in the first flight-scale design optimization of active flow control on an aircraft's vertical tail.

DEVELOPMENT

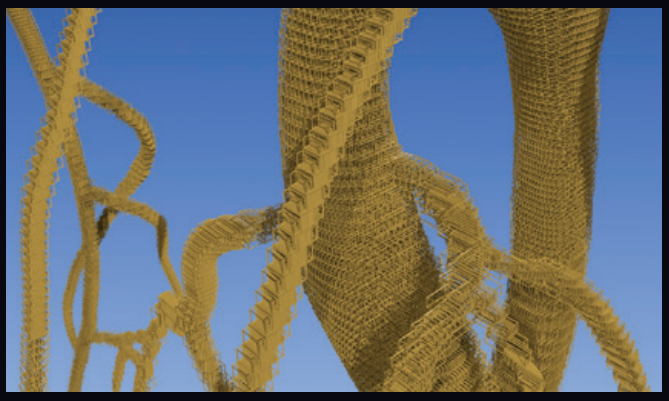
The scalable in situ data analysis, visualization, and compression for partial differential equations involved in this work will stress Aurora's underlying deep learning software and system characteristics. The project's data-intensive workflow, which incorporates uncertainty quantification and multifidelity modeling, will benefit from the system's I/O hardware.

DATA/LEARNING METHODS

Regression, uncertainty quantification, advanced workflows, advanced statistics, reduced/surrogate models, in situ visualization and analysis, and image and signal processing



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: CERN*



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*

Simulating and Learning in the ATLAS Detector at the Exascale

PI James Proudfoot
INST Argonne National Laboratory
SFTWR AthenaMT, Root, workflows, containers, TensorFlow

SCIENCE

This project will enable new physics discoveries by developing exascale workflows and algorithms that meet the growing computing, simulation and analysis needs of the ATLAS experiment at CERN's Large Hadron Collider.

DEVELOPMENT

The ATLAS software stack's diverse compute and analysis kernels will stress Aurora's deep learning software and hardware characteristics. An example of one key issue is the precision required by physics generators to match experimental statistics when comparing theory to experiment. The project's use of machine learning for reconstruction provides a novel use case that will likely leverage graph convolutions. This work will help to prepare Aurora for the computing needs of other large-scale experiments in high energy physics.

DATA/LEARNING METHODS

Classification, clustering, dimensionality reduction, advanced workflows, advanced statistics, image and signal processing, and databases

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

PI Amanda Randles
INST Duke University and Oak Ridge National Laboratory
SFTWR HARVEY, SENSEI, VTK

SCIENCE

The research team will develop computational models to provide detailed analysis of the role key biological parameters play in determining tumor cell trajectory in the circulatory system.

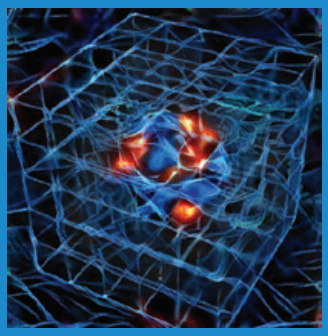
DEVELOPMENT

This project will stress and prepare data analysis and visualization frameworks for Aurora. Its complex, data-intensive workflows, which couple multiscale simulations and *in situ* analysis, are expected to benefit from the system's I/O hardware.

DATA/LEARNING METHODS

Advanced workflows, reduced/surrogate models, *in situ* visualization and analysis, and image and signal processing

Learning Projects



Researchers will couple machine learning and lattice QCD simulations to advance the study of nuclei. This artistic rendering was created with deepart.io.
Image: William Detmold and Phiala Shanahan, Massachusetts Institute of Technology

LEARNING

Machine Learning for Lattice Quantum Chromodynamics

PI	William Detmold
INST	Massachusetts Institute of Technology
SFTWR	MLHMC, USQCD libraries, Spearmint, TensorFlow, HDF5, MongoDB

SCIENCE

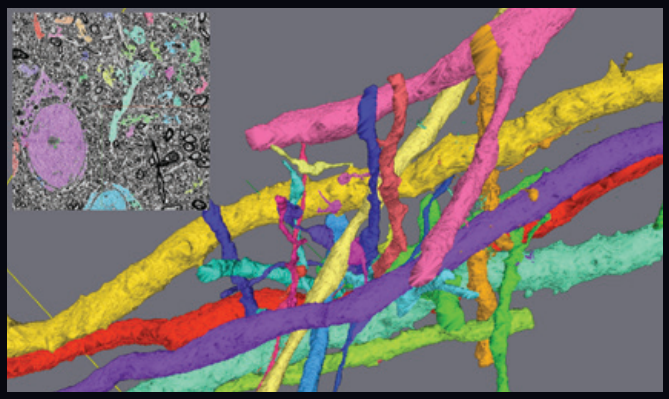
By coupling advanced machine learning and state-of-the-art physics simulations, this project will provide critical input for experimental searches aiming to unravel the mysteries of dark matter while simultaneously providing insights into fundamental particle physics.

DEVELOPMENT

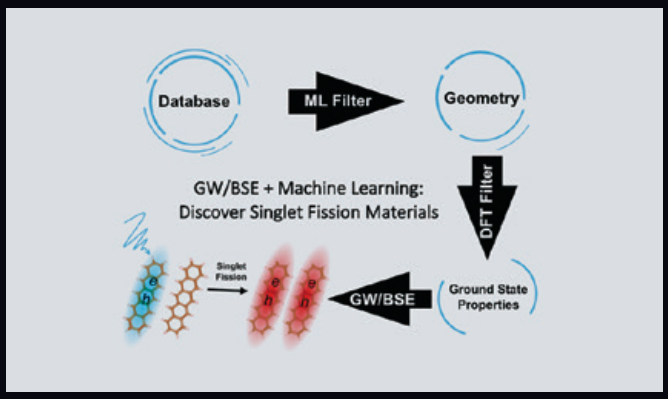
This project's novel machine learning models will stress Aurora's deep learning architecture and software stack at scale. Its workflow coupling machine learning (including deep reinforcement learning and hyperparameter optimization) and simulation could benefit from the system's I/O hardware.

DATA/LEARNING METHODS

Classification, regression, reinforcement learning, clustering, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, and databases



Neurons rendered from the analysis of electron microscopy data. The inset shows a slice of data with colored regions indicating identified cells. Tracing these regions through multiple slices extracts the sub-volumes corresponding to anatomical structures of interest. *Image: Nicola Ferrier, Narayanan (Bobby) Kasthuri, and Rafael Vescovi, Argonne National Laboratory*



A schematic illustration of the project's workflow. *Image: Noa Marom, Carnegie Mellon University*

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI Nicola Ferrier
INST Argonne National Laboratory
SFTWR TensorFlow, Horovod, flood-fill networks, AlignTK, Tomosaic

SCIENCE

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.

DEVELOPMENT

Compute-intensive and data-parallel deep learning models, flood-fill networks (FNN), together with large and complex data and image processing needs will stress the system's deep learning hardware/software and communication fabric. The near-real-time coupling of supercomputing resources and experiments provides a novel use case that will benefit future work on Aurora.

DATA/LEARNING METHODS

Classification, regression, clustering, uncertainty quantification, advanced workflows, advanced statistics, image and signal processing, and graph analytics

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

PI Noa Marom
INST Carnegie Mellon University
SFTWR SISSO, Bayesian optimization, BerkeleyGW, Quantum Expresso

SCIENCE

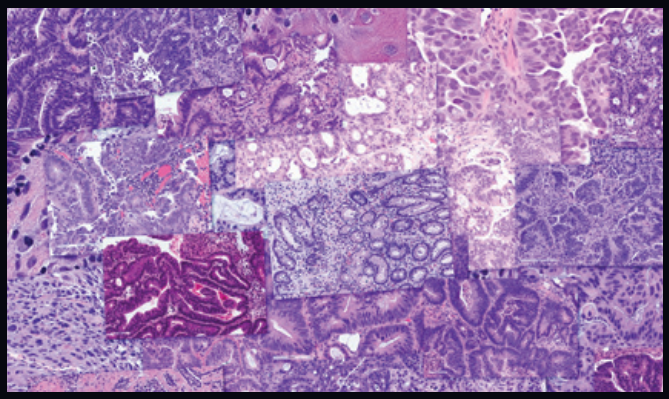
By combining quantum-mechanical simulations with machine learning and data science, this project will harness Aurora's exascale power to revolutionize the computational discovery of new materials for more efficient organic solar cells.

DEVELOPMENT

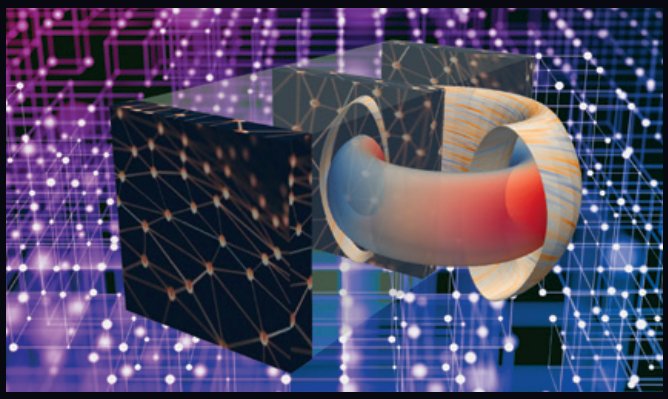
The use of feature selection and Bayesian optimization algorithms at scale will stress Aurora's deep learning stack. The project's workflow, which couples simulation, data, and learning methods, is expected to benefit from Aurora's I/O hardware.

DATA/LEARNING METHODS

Classification, regression, clustering, uncertainty quantification, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, and databases



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*



The team's Fusion Recurrent Neural Network uses convolutional and recurrent neural network components to integrate both spatial and temporal information for predicting disruptions in tokamak plasmas. *Image: Julian Kates-Harbeck, Harvard University; Eliot Feibush, Princeton Plasma Physics Laboratory*

Virtual Drug Response Prediction

PI Rick Stevens
INST Argonne National Laboratory
SFTWR CANDLE, Keras, TensorFlow

SCIENCE

Utilizing large-scale data frames and a deep learning workflow, researchers will enable billions of virtual drugs to be generated and screened singly and in numerous combinations, while predicting their effects on tumor cells. This approach aims to dramatically accelerate successful drug development and provide new approaches to personalized cancer medicine.

DEVELOPMENT

Novel models, including generative models and autoencoders, will stress the system's deep learning hardware and software stack. The project's use of data-parallel training and parallel inference, together with hyperparameter optimization, will significantly stress Aurora's communication fabric. This work also has the potential to use the system's I/O hardware to stage data for training and inference.

DATA/LEARNING METHODS

Classification, regression, clustering, uncertainty quantification, dimensionality reduction, advanced workflows, and image and signal processing

Accelerated Deep Learning Discovery in Fusion Energy Science

PI William Tang
INST Princeton Plasma Physics Laboratory
SFTWR Fusion Recurrent Neural Net (FRNN), Keras, TensorFlow

SCIENCE

This project will use deep learning and artificial intelligence methods to improve predictive capabilities and mitigate large-scale disruptions in burning plasmas in tokamak systems, such as ITER.

DEVELOPMENT

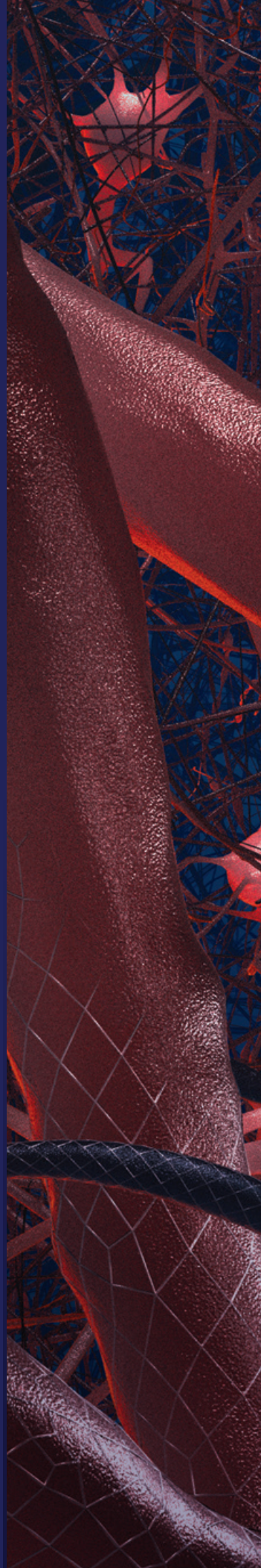
The FRNN software stack will stress the system's deep learning capabilities and software stack. Large data-parallel training and hyperparameter optimization requirements will stress Aurora's communication fabric and stand to benefit from the system's I/O hardware.

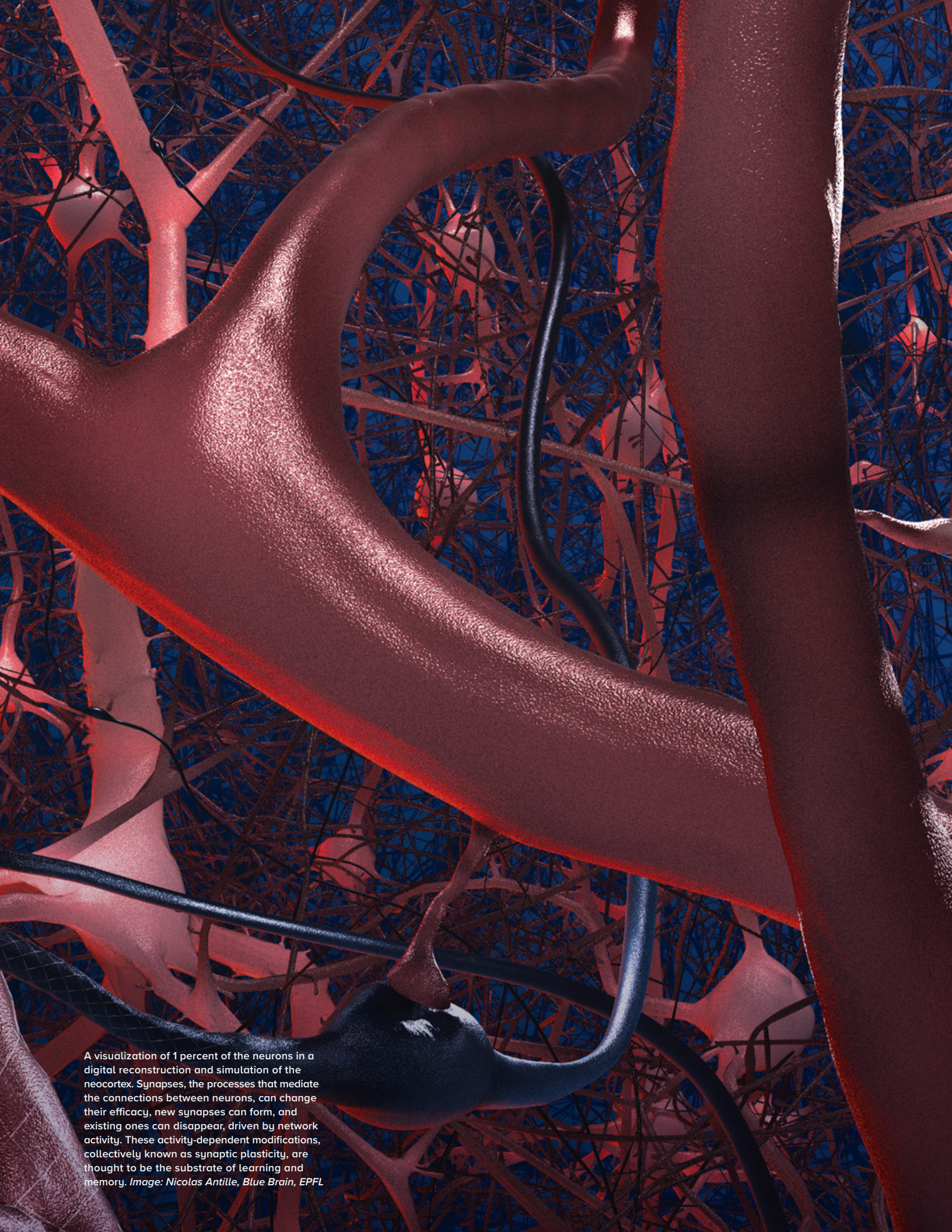
DATA/LEARNING METHODS

Classification, regression, clustering, and dimensionality reduction

GROWING THE HPC COMMUNITY

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





A visualization of 1 percent of the neurons in a digital reconstruction and simulation of the neocortex. Synapses, the processes that mediate the connections between neurons, can change their efficacy, new synapses can form, and existing ones can disappear, driven by network activity. These activity-dependent modifications, collectively known as synaptic plasticity, are thought to be the substrate of learning and memory. *Image: Nicolas Antille, Blue Brain, EPFL*

Partnering with Industry to Enable High-Impact Research

The ALCF's industry partnerships help to strengthen the nation's innovation infrastructure and expand the use of supercomputing resources for technological and engineering advances.

Leadership computing systems like Theta and Mira enable industry users to tackle multifaceted problems too complex for traditional clusters to address.

ALCF supercomputers—equipped with advanced simulation, data, and learning capabilities—help companies accelerate R&D efforts for applications that include, among others, combustion engines, novel materials for medicine, and fusion energy devices.

Access to ALCF systems and expertise allows industry researchers to create higher-fidelity models, make predictions with greater accuracy, and rapidly analyze massive quantities of data. Such results permit companies to achieve critical breakthroughs faster by verifying uncertainties and drastically reducing—or even eliminating—the need to build multiple prototypes.

Industry partnerships with the ALCF consequently help to strengthen the nation's infrastructure for innovation and increase competitiveness therein.

To expand and deepen this impact, the ALCF Industry Partnerships Program, led by David Martin, focuses on growing the facility's community of industry users by engaging prospective companies of all sizes—from start-ups to Fortune 500 corporations—that could benefit from the facility's resources and expertise.

The ALCF works closely with other Argonne user facilities and divisions, including the Technology Development and Commercialization Division, to create opportunities for collaboration throughout the laboratory. Through this approach, the ALCF is able to present a more complete picture of the laboratory's many resources, resulting in broader engagements across Argonne.

Martin also serves as co-executive director of the DOE's Exascale Computing Project Industry Council, an external advisory group of senior executives from prominent U.S. companies who are passionate about bringing exascale computing to a wide range of industry segments.

DRIVING INNOVATION FOR U.S. INDUSTRY

The following project summaries illustrate how companies are using ALCF resources to advance their R&D efforts.

Kinetic Simulation of Field-Reversed Configuration Stability and Transport

PI Sean Dettrick
INST TAE Technologies

With this INCITE project, researchers from TAE Technologies are performing simulations on Theta to accelerate their experimental research program aimed at developing a clean, commercially viable, fusion-based electricity generator. The team will use the simulation results to optimize a device for studying the confinement of energy with high plasma temperatures, and to inform the design of a future prototype reactor.

Advancing Computer-Aided Drug Design

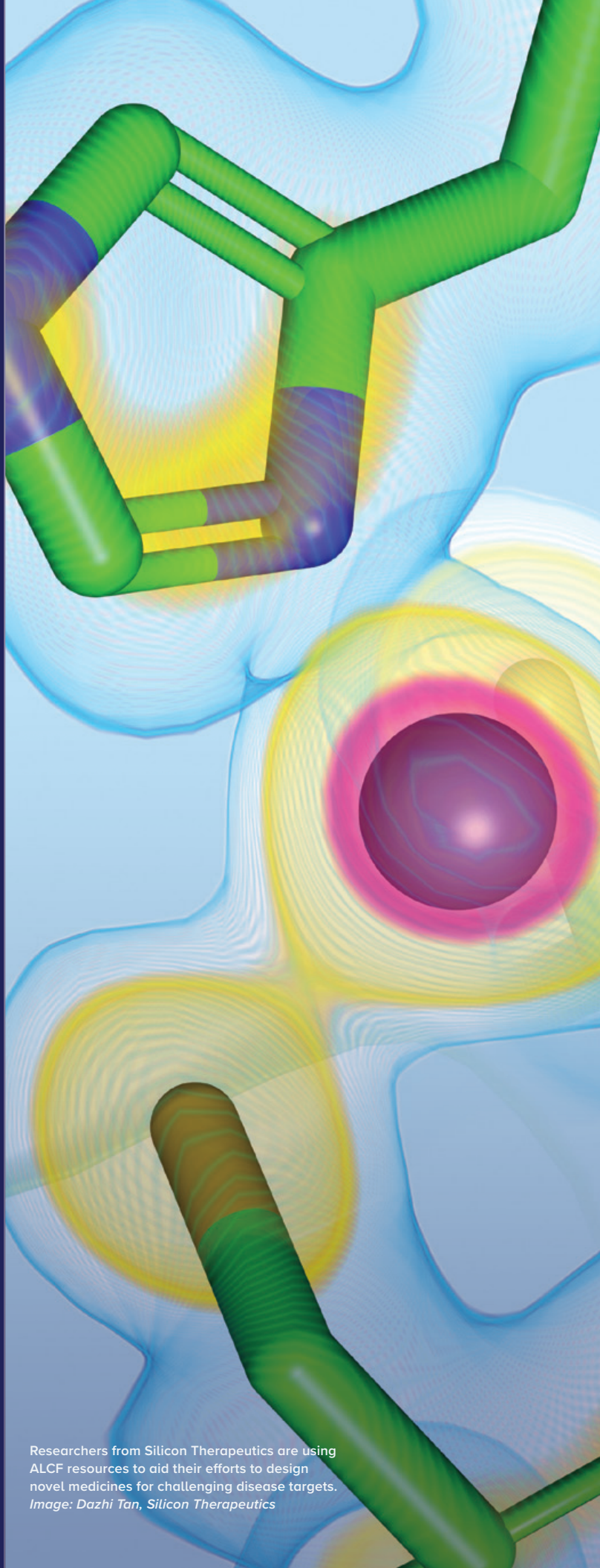
PI Vipin Sachdeva
INST Silicon Therapeutics

Researchers from Silicon Therapeutics are using an ALCF Director's Discretionary allocation to perform important tasks related to their physics-based drug design platform, including scientific validation, parameter optimization, and HPC performance benchmarking. This work is helping to advance the company's drug discovery work and will also be published to benefit the broader computer-aided drug design community.

Enabling Multiscale Physics for Industrial Design Using Deep Learning Networks

PI Rathakrishnan Bhaskaran
INST GE Global Research

GE Global Research's ALCF Data Science Program project is focused on leveraging machine learning and large datasets generated by wall-resolved large-eddy simulations to develop data-driven turbulence models with improved predictive accuracy. The researchers will apply this approach to turbomachinery, such as a wind turbine airfoil, demonstrating the impact that deep learning can have on industrial design processes for applications in power generation, aerospace, and other fields.



Researchers from Silicon Therapeutics are using ALCF resources to aid their efforts to design novel medicines for challenging disease targets. *Image: Dazhi Tan, Silicon Therapeutics*

Shaping the Future of Supercomputing

ALCF researchers are at the forefront of numerous strategic activities that aim to push the boundaries of what's possible with high-performance computing.

As home to some of the world's most powerful computing resources, the ALCF breaks new ground with the development and deployment of each new supercomputer.

ALCF staff members, collaborating with the researchers who use leadership-class systems to pursue scientific breakthroughs, are involved in the development and testing of new HPC hardware and software. This unique position the ALCF occupies affords the facility an important perspective on the trends, methods, and technologies that will define the future of supercomputing.

Leveraging this knowledge and expertise, ALCF researchers contribute to many forward-looking activities aimed at advancing the use of supercomputers for discovery and innovation.

These efforts include organizing workshops and meetings on topics like quantum computing and computational neuroscience; engagement in leading user groups and conferences; and contributions to the development of standards, benchmarks, and technologies that help propel continued improvements in supercomputing performance.

Ray Loy, ALCF lead for training, debuggers, and math libraries, delivers a talk at the ALCF Computational Performance Workshop, an annual event that connects facility users with staff and industry experts for hands-on assistance in boosting code performance.

Community Activities

Computational Neuroscience Workshop

In late August, Argonne and Northwestern University jointly hosted a workshop on computational neuroscience to foster collaborations between researchers and to discuss new ideas for research opportunities, including routes to successful proposals for ALCF allocations.

Exascale Computing Project

The ALCF is a key contributor to the DOE's Exascale Computing Project (ECP), a multi-lab initiative aimed at accelerating the development of a capable exascale computing ecosystem. Several ALCF researchers are engaged in ECP-funded projects in application development, software development, and hardware technology. ALCF computing resources, particularly Theta, allow ECP research teams to pursue development work at a large scale. In the workforce development space, the ECP now funds the annual Argonne Training Program on Extreme-Scale Computing (ATPESC), which is organized and managed by ALCF staff.

HPC Standards, Benchmarks, and Technologies

ALCF staff members remain actively involved in the development of standards, benchmarks, and technologies that help drive continued improvements in supercomputing performance. Staff activities include contributions to the C++ Standards Committee, Cray User Group, HPC User Forum, Intel eXtreme Performance Users Group, MPI Forum, OpenMP Architecture Review Board, OpenMP Language Committee, and Open Scalable File Systems (OpenSFS) Board.

Intel eXtreme Performance Users Group

David Martin of the ALCF currently serves as president of the Intel eXtreme Performance Users Group (IXPUG), whose mission is to provide a forum for exchanging information to enhance the usability and efficiency of scientific and technical applications running on large-scale HPC systems that use the Xeon Phi processor, like Theta. IXPUG held eight significant meetings in 2018, in addition to workshops and birds-of-a-feather sessions at the International Supercomputing Conference and at SC. ALCF staff organized and hosted the 2018 IXPUG In Situ Visualization Hackathon in July.

Argonne's national Quantum Computing Workshop included a wide range of presentations and hands-on sessions that trained attendees on how to work with quantum simulators.

Lustre Users Group Conference

In April, the ALCF and Globus hosted the 2018 Lustre User Group (LUG) conference at Argonne National Laboratory. The event connected 130 Lustre users from around the world, providing the opportunity to learn from each other and share best practices. Kevin Harms and Paul Coffman of the ALCF were among the presenters at this year's conference. As an active member of OpenSFS, the ALCF has been a key contributor to the continued advancement of Lustre, an open-source, parallel file system that supports many of the requirements of leadership-class supercomputing environments.

Performance Portability

The ALCF continued its collaboration with NERSC and OLCF to operate and maintain a website dedicated to enabling performance portability across the DOE Office of Science HPC facilities (performanceportability.org). The website serves a documentation hub and guide for applications teams targeting systems at multiple computing facilities. Content includes an overview of the facilities' systems and software environments, information on various performance analysis tools, and case studies that detail promising performance-portable programming approaches.

Quantum Computing Training

ALCF staff members organized the Quantum Computing Workshop, held at Argonne over three days in July and featuring more than 150 speakers from the University of Chicago, Intel, Google, Rigetti, and DOE national laboratories. The workshop—designed to serve as an incubator for future collaborations—taught attendees about tools available for simulating quantum computers while also informing them about the quantum computing programs offered by participating institutions, highlighted promising research opportunities, and presented state-of-the-art domain research.

SC18

With over 60 of its researchers attending, Argonne had a prominent presence at this year's International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC18), held in Dallas, Texas. Argonne researchers presented technical papers; delivered talks; and participated in workshops, birds-of-a-feather sessions, panel discussions, and tutorials. ALCF staff organized an annual lunch with industry HPC users—including representatives from Boeing, General Motors, and General Electric—to discuss potential partnerships and strategies to improve their efficacy.

Engaging Current and Future HPC Users

The ALCF provides training and outreach opportunities that prepare researchers for efficient use of its leadership computing systems, while also cultivating a diverse and skilled HPC community for tomorrow.

Outreach to the facility's user community is focused on providing expert-guided training for the growing array of computational resources, methods, and services available at the ALCF to support the advancement of scientific discovery.

In 2018, the ALCF hosted a number of events intended to optimize use of its systems, including a new annual series of hands-on workshops aimed at improving the performance of simulation, data science, and machine learning applications; interactive videoconferences to connect users and developers from industry leaders such as Intel; and webinars designed to support Early Science Program teams.

The ALCF also supports a wide variety of outreach activities directed at students, with staff members volunteering to engage participants. Multi-day camps centered around programming and big data visualization, as well as events like Hour of Code and SC's Student Cluster Competition, spark students' interest in different aspects of scientific computing and introduce them to exciting career possibilities.

Additionally, the ALCF's annual summer student program gives college students the opportunity to work side-by-side with staff members on real-world research projects and utilize some of the world's most powerful supercomputers, collaborating in areas like computational science, system administration, and data science.

Argonne's Big Data and Visualization Camp is designed to teach high school students how to gain insights from vast amounts of data.

Inspiring Students

Big Data and Visualization Camp

In July, Argonne launched a new three-day Big Data and Visualization Camp for area high school students. Led by ALCF Director Michael Papka and several ALCF colleagues and organized by Argonne's Educational Programs Office, the camp is designed to teach attendees how visualization helps researchers gain insights into massive amounts of data. The students used Python to program visualization tools and worked with data obtained from Argonne and the University of Chicago's urban sensor project, Array of Things.

CodeGirls@Argonne Camp

In June, 25 seventh- and eighth-grade girls attended Argonne's two-day camp that teaches the fundamentals of coding in the Python programming language. The attendees also met and interviewed five Argonne scientists, and toured the ALCF's machine room and visualization lab.

Hour of Code

As part of the national Computer Science Education Week (CSEdWeek) in December, several ALCF staff members visited various Chicago and suburban classrooms to give talks and demos intended to spark interest in computer science. Working with students in grades from kindergarten to high school, the volunteers led a variety of activities designed to impart the basics of coding. CSEdWeek was established by Congress in 2009 to raise awareness about the need for greater computer science education.

National Science Bowl

As part of the Cyber Challenge at DOE's 2018 National Science Bowl in April, the ALCF's Ti Leggett teamed up with Carolyn Lauzon of DOE's Advanced Scientific Computing Research Program to present a demo on HPC and cyber security to a group of middle school students. Leggett also participated in workshops designed to help teachers prepare students for the future of computing.

The CodeGirls@Argonne camp is designed to immerse middle school students in computer science and introduce them to potential STEM career paths.

SC18 Student Cluster Competition

The ALCF co-sponsored the Chicago Fusion team in the Student Cluster Competition at SC18, an annual event that challenges student teams to assemble a working cluster on the conference exhibit floor and demonstrate its performance using real scientific applications and benchmarks. Chicago Fusion was comprised of students from the Illinois Institute of Technology (IIT). With financial and technical support provided by Argonne, IIT, Intel, NVIDIA, Mellanox, and the National Science Foundation, the team earned fourth place in the High Performance Linpack (HPL) benchmark portion of the challenge. To prepare for the competition, ALCF researchers William Scullin and Ben Allen worked closely with the students to provide logistical, setup, and application support.

Summer Coding Camp

Over five days in July, ALCF staff members taught and mentored 30 local high school students at Argonne's Summer Coding Camp. The camp curriculum promotes problem-solving and teamwork skills through interactive coding activities, including working with the Python language and programming a robot. The camp is a joint initiative of the ALCF and Argonne's Educational Programs Office.

Summer Student Program

Every summer, the ALCF opens its doors to a new class of student researchers who work alongside staff mentors to tackle research projects that address issues at the forefront of scientific computing. This year, the facility hosted 45 students ranging from undergraduates to PhD candidates. From exploring the potential of quantum computing to visualizing system logs of HPC systems, many of this year's interns had the opportunity to gain hands-on experience with some of the most advanced computing technologies in the world. The summer program culminated with a series of special seminars that allowed the students to present their project results to the ALCF community.

Women in STEM

For the laboratory's annual Introduce a Girl to Engineering (IGED) event in February, approximately 100 local eighth graders were paired with Argonne researchers during presentations and hands-on activities focused on science, technology, engineering, and mathematics (STEM) careers. Event co-chair Liza Booker and many other ALCF staff members participated as speakers, mentors, and supervisors throughout the day's activities. ALCF staff members also served in various roles at the 31st Annual Science Careers in Search of Women Conference, hosted by Argonne in April, and contributed to Argonne's Women in Science group, Women in Statistics and Data Science, and the Grace Hopper Celebration of Women in Computing.

Training Users

ALCF Computational Performance Workshop

Held in May, this annual scaling workshop is a cornerstone of the ALCF's user outreach efforts, attracting prospective INCITE users for talks and hands-on application tuning on Mira and Theta. Attendees work with ALCF computational scientists, performance engineers, data scientists, and visualization experts, as well as tool and debugger vendors, with the goal of submitting INCITE project proposals. Roughly 40 percent of attendees who submitted a proposal were awarded INCITE or ALCC allocations.

ALCF Getting Started Videoconferences

The ALCF conducts several "Getting Started" videoconferences throughout the year to help users get their projects up and running on Mira and Theta. These virtual, hands-on sessions cover system specs, code building, storage, operating and file systems, compilers, tools, queues, and other topics.

ATPESC 2018

A two-week training program funded by the Exascale Computing Project, the ALCF held the sixth annual Argonne Training Program on Extreme-Scale Computing (ATPESC) this summer. The highly competitive program, aimed at early career researchers and aspiring computational scientists, teaches the skills, approaches, and tools necessary to design, implement, and execute computational science and engineering applications on leadership-class computing systems through seven learning tracks. Leaders of the research and HPC communities deliver technical lectures and guide hands-on laboratory sessions, with 73 attendees participating this year. To extend ATPESC's reach, ALCF staff produces and uploads video playlists to Argonne's YouTube training channel.

Aurora Early Science Program Training Series

The ALCF kicked off a series of web-based training events exclusively for Aurora Early Science Program project teams. The training events are designed to provide instruction and hands-on exercises on topics and tools relevant to current production machines, with an emphasis on data intensive and machine learning subjects. The first webinar in the series covered the effective use of Python on ALCF systems.

The ALCF's Simulation, Data, and Learning Workshops enabled enabled attendees to work directly with staff and industry experts to hone their abilities using tools, systems, and frameworks that can accelerate scientific computing on ALCF systems.

Best Practices for HPC Software Developers

In 2018, the ALCF, OLCF, NERSC, and the Exascale Computing Project continued their collaboration with the Interoperable Design of Extreme-Scale Application Software (IDEAS) project to deliver a series of webinars—Best Practices for HPC Software Developers—to help users of HPC systems carry out their software development more productively. Webinar topics included Jupyter and HPC, open source best practices, software citation, and software sustainability.

Many-Core Developer Sessions

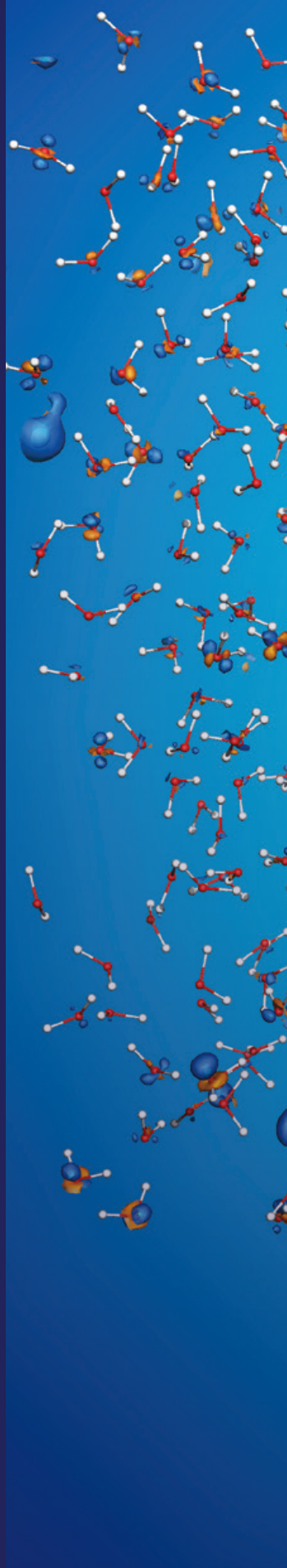
To help support and grow the Theta user base, the ALCF introduced a tutorial series and a live-presentation webinar aimed at efficient use of the manycore system. The "Many-Core Tools and Techniques" tutorial series has so far covered such topics as architectural features, tuning techniques, analysis tools, and software libraries. The "Many-Core Developer Sessions" webinar series intends to foster discussion between actual developers of emerging many-core hardware and software and the technology's early users. Speakers in the webinars have included developers from Intel and Allinea (ARM), covering topics like AVX-512, math kernel library, Vtune, TensorFlow, and debugging.

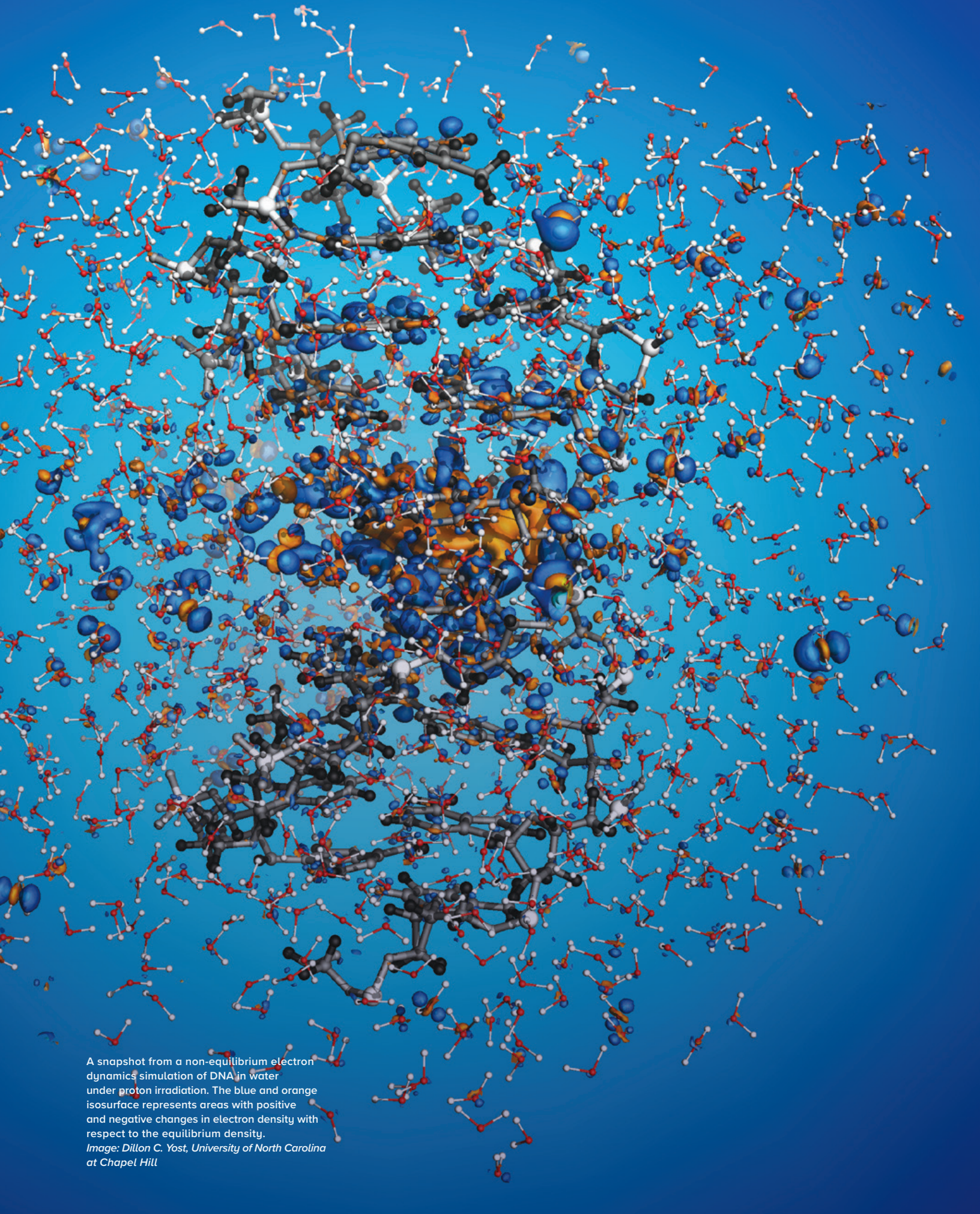
Simulation, Data, and Learning Workshops

The ALCF hosted two hands-on workshops, one in February and another in October, to help users improve the performance and productivity of simulation, data science, and machine learning applications on ALCF systems. Attendees worked directly with ALCF staff and industry experts, learning how to use data science tools and frameworks at scale on ALCF systems. Topics covered included machine learning frameworks like TensorFlow, Horovod, and Pytorch, as well as workflow management services, to advance data science projects. The workshop will recur annually.

EXPERTISE AND RESOURCES

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





A snapshot from a 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

The 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.

Staff News

Laural Briggs (right) receives the 2018 SCSW Founders Award from Emily Zvolanek (left), program initiator of Argonne's Women in Science and Technology Program.

KUMARAN RECEIVES 2018 SPEC PRESIDENTIAL AWARD

Kalyan Kumaran, Director of Technology at the ALCF, was the 2018 recipient of the Standard Performance Evaluation Corporation's (SPEC's) highest honor, the Presidential Award, for his contributions to SPEC as chair of the High-Performance Group (SPEC/HPG). Also serving on the SPEC CPU committee and elected member of the SPEC Board of Directors, Kumaran expanded participation in the benchmark development process by bringing universities and major research laboratories into the fold. All three current HPG benchmarks for modern high-performance computing systems were developed under his leadership.

HARMS WINS R&D 100 AWARD

Kevin Harms, ALCF Lead for I/O Libraries and Benchmarks, and colleagues from Argonne's Mathematics and Computer Science Division—Philip Carns, Robert Latham, Robert Ross, and Shane Snyder—received an R&D 100 Award for their work developing the Darshan software package. Capable of running on some of the world's largest supercomputers—including the Intel-Cray and IBM Blue Gene/Q systems housed at the ALCF—Darshan enables researchers to investigate and tune the I/O behavior of complex high-performance computing applications.

MESSINA SELECTED FOR DISTINGUISHED SERVICE AWARD

Paul Messina, Director of Argonne's Computational Science Division, was selected as the 2018 recipient of the CRA Distinguished Service Award in recognition of his numerous contributions to the advancement of high-performance computing. Impacting not just the research community but U.S. policy, Messina led the U.S. Department of Energy Exascale Computing Project, accelerating delivery of the country's first exascale system.

BRIGGS RECEIVES SCSW FOUNDERS AWARD

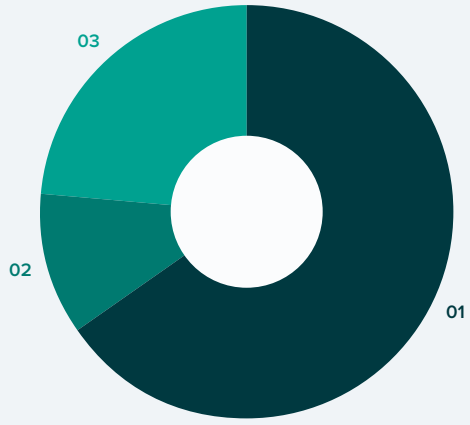
Laural Briggs, Argonne nuclear engineer and advisor to the ALCF, received the 2018 Science Careers in Search of Women (SCSW) Founders Award for her dedication to organizing and participating in various outreach and mentoring activities at the laboratory. In May, Briggs retired from Argonne, where she had worked since 1977.

Staff Spotlights

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

With a shared passion for research and innovation, ALCF staff members are helping to shape the future of supercomputing. The following pages highlight six staff members and some of their notable contributions in 2018.

ALCF STAFF NUMBERS



01 Staff Members

95

02 Postdoctoral Researchers

16

03 Summer Students

34

THOMAS APPLENCOURT
Computational Scientist

COLLEEN BERTONI
Computational Scientist

Thomas, as a computational scientist at the ALCF, chiefly helps the facility augment its expertise in innovative hardware. This work involves executing performance assessments not just of the hardware but of its associated compilers as well, in addition to evaluating and providing feedback about the programming model employed in next-generation exascale systems.

Thomas supervises a doctoral student whose work concerns maximizing the performance of data-flow graphs and developing efficient algorithms designed to facilitate this goal. Engaged in ALCF outreach efforts, Thomas also advised a summer student who, adopting a special algorithm from quantum chemistry intended to improve the accuracy of the method's input, used quantum Monte Carlo to study problems in solid-state physics.

Colleen first came to the ALCF as a summer student in 2016 to work on the facility's RAM Area Network project, which seeks to treat RAM as a schedulable resource in compute clusters. After earning her PhD in chemistry from Iowa State University, she returned to Argonne in 2017 as the recipient of the ALCF's Margaret Butler Fellowship in Computational Science. In this role, she focused on improving the performance and accuracy of a new quantum chemistry code that can be used to calculate the properties of complex chemical systems.

In July 2018, she joined the ALCF fulltime as a member of Performance Engineering, where she participated in several non-recurring engineering groups and presented material on preparing applications for exascale at several Aurora meetings. Colleen instructed attendees in the use of Cray performance tools at the May 2018 Computational Performance workshop, while also contributing to a paper for one of the annual IEEE International Parallel and Distributed Processing Symposium Workshops as well as to a paper published in *Computing in Science and Engineering*.

Colleen continues to remain active as a chemist through her computational work, aiding development of the quantum chemistry software package GAMESS and open-source codes such as VALENCE.

TAYLOR CHILDERS
Computer Scientist

GORDON MCPHEETERS
HPC Systems Administrator—File Systems

Taylor, formerly a physicist in Argonne's High Energy Physics Division, joined the ALCF in January 2018, following four years spent as a principal investigator on ASCR Leadership Computing Challenge and ALCF Data Science Program projects designed to improve simulations for the Large Hadron Collider's ATLAS experiment on ALCF resources. Since then he has collaborated with ALCF researchers to develop the Balsam workflow management service for helping users optimize job submissions on Mira, Theta, and other supercomputers; the service is now publicly available to users and was presented at the Supercomputing Conference in 2017 and 2018. He tested the stability and usability of Singularity, the new software container framework installed on Theta, which was necessary to achieve linear scaling of ATLAS simulations.

Taylor continues to support supercomputing efforts in this domain via a newly awarded Early Science Program project, which will investigate the use of machine learning methods as replacements for compute-intensive detector reconstruction algorithms, as well as a SciDAC proposal to reengineer perturbative quantum chromodynamics simulations for supercomputers. Both projects target the 2021 deployment of the ALCF's exascale system, Aurora.

As the file system technical lead for HPC storage, Gordon McPheeters has been instrumental in architecting and supporting HPC storage facilities within the ALCF and the Joint Laboratory for System Evaluation. Gordon joined the ALCF from IBM, where he worked on GPFS parallel file system development.

Responsible for supporting the full lifecycle of project data, Gordon applies his depth of knowledge to enable projects to store and manage their research products. The systems he is responsible for include the parallel file system clusters for Mira, Theta, and Cooley. In his duties, he optimizes these systems for performance and stability, and consults projects on data management and assists with troubleshooting.

Gordon also lends his expertise to the Aurora project, as he excels at identifying, testing, and assessing emerging technologies. In this capacity he collaborates with vendors to test and evaluate the operational characteristics of future file system hardware and software designs.

JEFF NEEL
Cyber Security Engineer/HPC Systems Administrator

HARITHA SIDDABATHUNI SOM
User Experience Team Lead

Jeff is responsible for all security aspects of the ALCF's HPC machines and supporting systems. This means that vulnerability analysis, update monitoring, penetration testing of internal and external applications, incident response, and coordination with Argonne's Cyber Security Program Office all fall under his purview. While he initially joined Argonne as a research assistant, he has since worked to improve the security level of the ALCF by collaborating with Operations staff to identify issues and fix points of weaknesses in the facility's supercomputing environment and its ancillary systems.

Jeff is currently involved in the penetration testing of two internal applications, both of which are in their beta versions, to be made publicly available to ALCF users: the ALCF's new account and project management system (set to enter production in early 2019), and an iOS mobile application that will allow users to monitor machine status and receive notifications on queue depth. He has been crucial in helping to ensure the facility's new applications meet Argonne's security standards.

Haritha began her role with the ALCF in May 2017. Her day-to-day responsibilities include overseeing the ALCF User Experience team's efforts to manage user accounts, system access, technical support inquiries, and ramp-ups for the various ALCF allocation programs. Under her direction, the team has developed scripts and collaborated with other ALCF staff members to automate aspects of the project creation process, thereby reducing the organization and execution of certain core tasks from hours to minutes.

Haritha has contributed to projects critical to the future of the facility, including leading training and support preparations for the Early Science users of Aurora, the ALCF's future exascale system. She has also worked closely with ALCF software developers to plan and test the facility's new account and project management system ahead of its scheduled deployment in 2019.

In addition, Haritha is a member of Argonne National Laboratory's User Facilities Experience Group, where she assists in the research and recommendation of solutions to provide an improved user experience for researchers working at the laboratory's various user facilities. She also found time to volunteer at Argonne's Introduce a Girl to Engineering Day and CodeGirls events in 2018.

ALCF Computing Resources

The ALCF provides users with access to supercomputing resources that are significantly more powerful than systems typically used for open scientific research.

Mira and Theta are the engines that drive scientific discoveries and engineering breakthroughs at the ALCF. At around 10 petaflops each, the facility's two production systems are among the fastest supercomputers in the world for open science.

Supporting systems—Cetus, Vesta, and Iota—are used for debugging and test and development work.

Cooley, the facility's visualization cluster, helps transform computational data into high-resolution images, videos, and animations, helping users to better analyze and understand simulations produced by ALCF supercomputers.

The ALCF's supercomputing environment also includes advanced data storage systems and networking capabilities.

Additionally, Argonne's Joint Laboratory for System Evaluation (JLSE) maintains a range of leading-edge hardware and software environments to enable researchers to evaluate and assess next-generation platforms.

THEORY AND COMPUTING SCIENCES BUILDING

ALCF computing resources, along with other Argonne computing systems, are housed in the Theory and Computing Sciences (TCS) Building's data center. The facility has 25,000 square feet of raised computer floor space and a pair of redundant 20 megavolt amperes electrical feeds from a 90 megawatt substation. The data center also features 3,950 tons of cooling capacity (two 1,300-ton chillers for Mira and two 675-ton chillers for air cooling at TCS).

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

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

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

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

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

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

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. The tape technology is currently undergoing an upgrade to replace LTO-6 tape drives with LTO-8 tape drives. The upgrade should ultimately provide up to 300 PB of effective storage (approximately five times the amount provided by the LTO-6 tapes).

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.

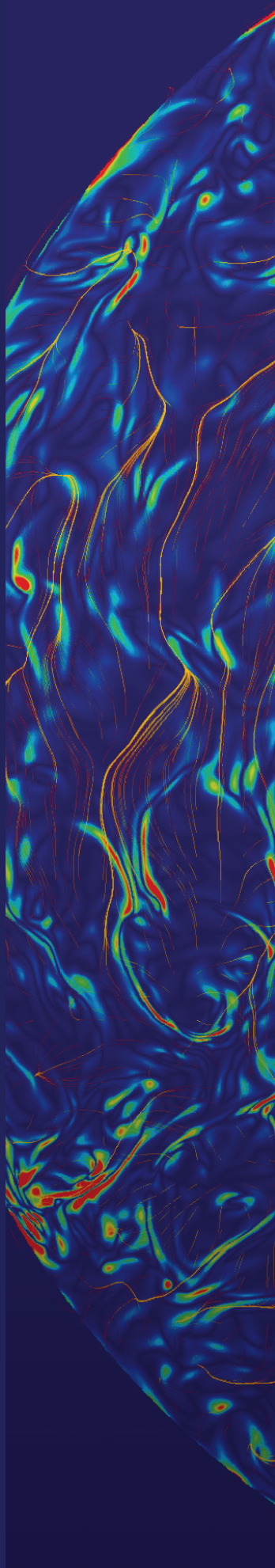
Testbeds

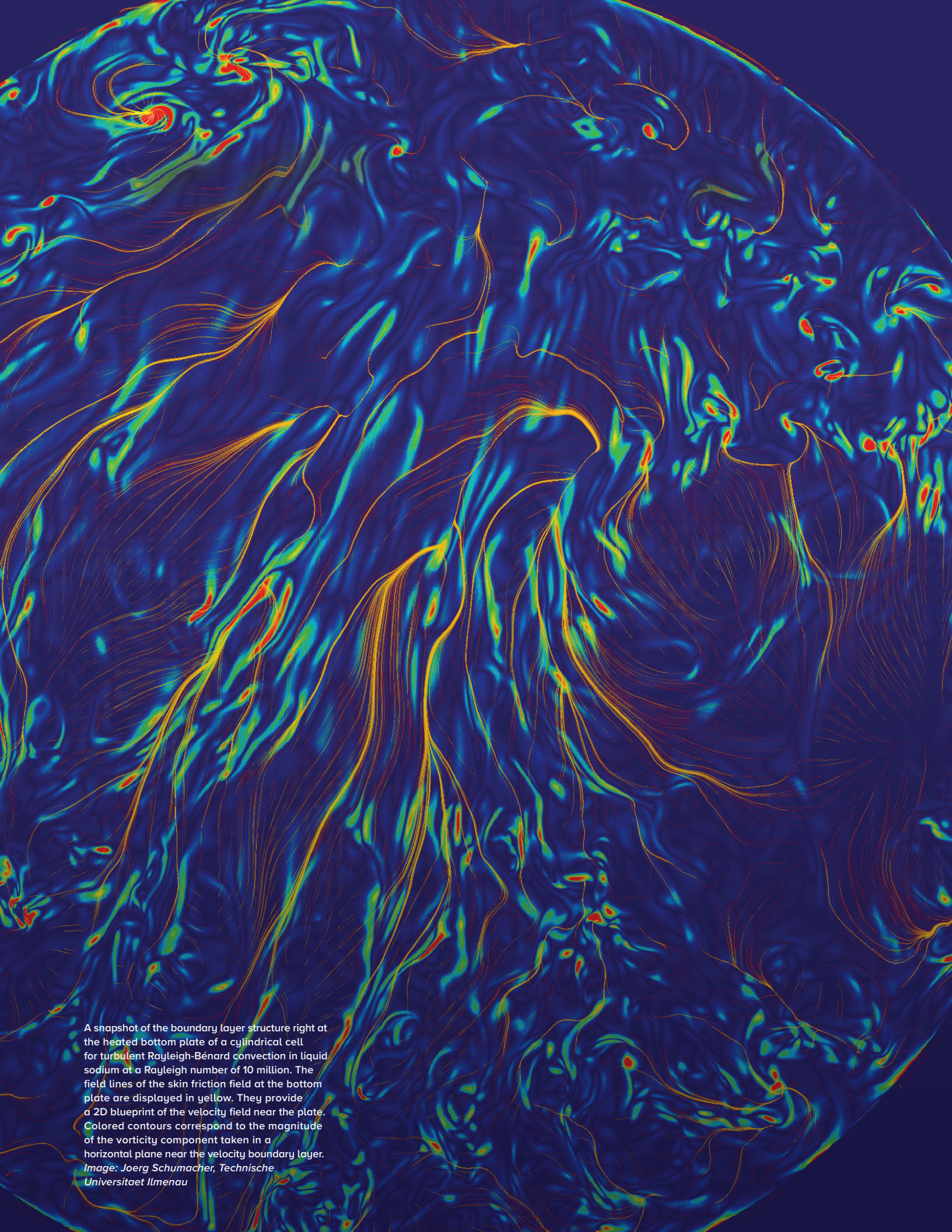
Through Argonne's Joint Laboratory for System Evaluation, the ALCF provides access to next-generation hardware and software to explore low-level experimental computer and computational science, including operating systems, messaging, compilers, benchmarking, power measurements, I/O, and new file systems.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

SCIENCE

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





A 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*

Awarding Compute Time on ALCF Resources

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

Researchers gain access to ALCF systems for computational science and engineering projects 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

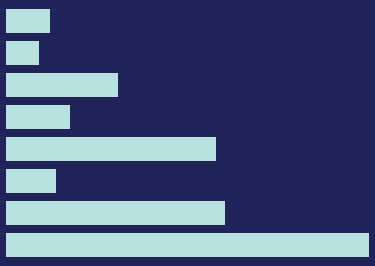
3.78B

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	

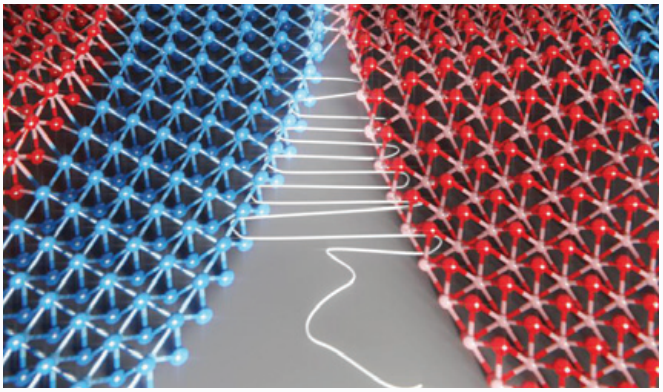


Note: ALCC data are from calendar year 2018.

Chemistry

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

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



Researchers have revealed a new technique to 'sew' two patches of crystals seamlessly together to create atomically thin fabrics. *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 finetuning of macroscopic properties including the optical and conductive. Results from this study were published in Science.

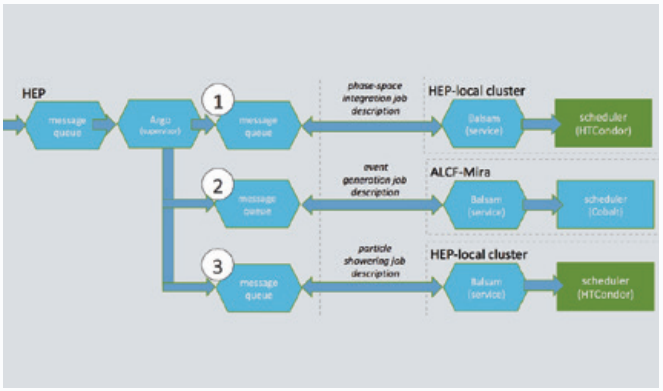
IMPACT

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
Saien Xie, Lijie Tu, Yimo Han, Lujie Huang, Kibum Kang, Ka Un Lao, Preeti Poddar, Chibeom Park, David A. Muller, Robert A. DiStasio Jr., and Jiwoong Park. "Coherent, atomically thin transition-metal dichalgocgenide superlattices with engineered strain," *Science* (March 2018), AAAS.

Balsam: Workflow Manager and Edge Service for HPC Systems

PI Thomas Uram, Taylor Childers
INST Argonne National Laboratory
HOURS DD, 250,000 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 high-performance computing (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

As part of an ALCC project, the ALCF-ATLAS effort 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 to run ensemble jobs on more than 1,000 Theta nodes for ECP, ADSP, and ESP projects, involving quantum chemistry, materials science, and studies of hyperparameter optimization in deep learning (DeepHyper).

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 ALCF opportunities to optimize job placement and possibly improve system utilization.

PUBLICATIONS

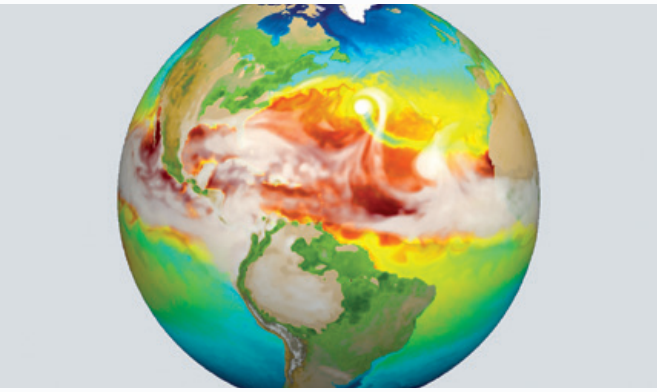
Childers, J.T., T. D. Uram, D. Benjamin, T. J. LeCompte, and M. E. Papka. "An Edge Service for Managing HPC Workflows." *Proceedings of the Fourth International Workshop on HPC User Support Tools - HUST'17* (2017).

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.

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 forty years.

APPROACH

The team made extensive use of Theta to run the recently released ES3M 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

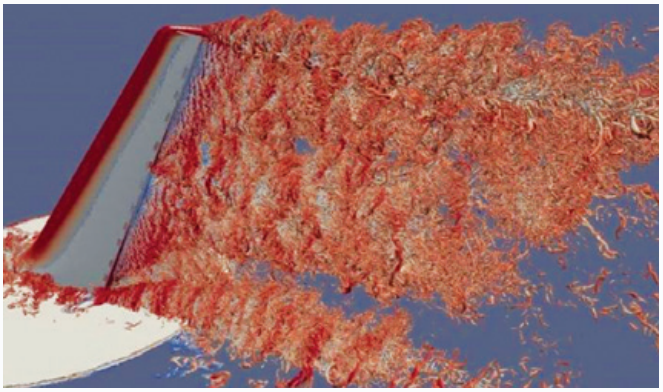
In addition to further advancing the predictive power of climate models and providing insight into the climatic effects of rapid changes in the earth's ice content, the ES3M simulations have the potential to answer how water resources and the hydrological cycle interact with the climate system on both 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.

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).

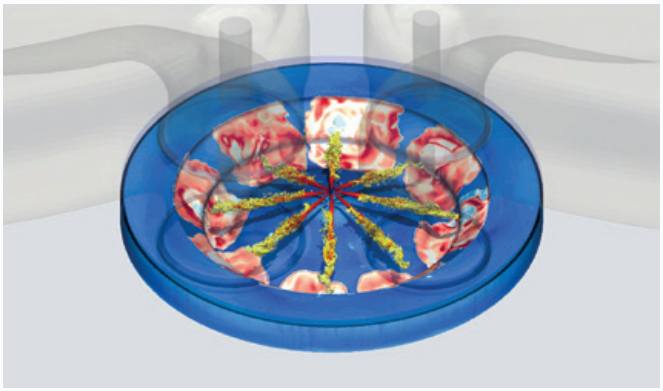
IMPACT

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

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

PI Pinaki Pal
INST Argonne National Laboratory
HOURS DD, 26.5 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 Services Company: Aramco Research Center–Detroit, and Convergent Science Inc. *Image: Roberto Torelli and Joseph A. Insley, Argonne National Laboratory; Yuanjiang Pei, Aramco Services Company: 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 Services Company: 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. Large ensembles of simulations were then performed spanning a wide engine design space on Mira supercomputer, based on design of experiments (DOE) approach. Thereafter, the piston geometry and engine operating conditions were optimized in a staged manner using a response surface method. In an earlier project with Convergent Science, Inc., ALCF staff helped to optimize the 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 over 3,000 high-fidelity engine design combinations in a matter of days, covering four different operating conditions, 256 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 indicated specific fuel consumption of up to 6.3 percent while meeting the future low criteria pollutants standard. The computational study allowed the team to narrow down the best-performing scenarios to a specific set 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 the carbon footprint of transportation.

PUBLICATIONS

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* (2017)

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* (2017)

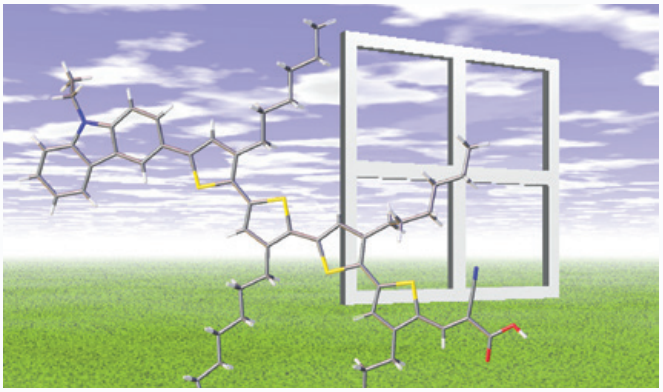
Moiz, A.A., P. Pal, D. Probst, Y. Pei, Y. Zhang, S. Som, and J. Kodavasal. "A Machine Learning-Genetic Algorithm (ML-GA) Approach for Rapid Optimization Using High-Performance Computing," *SAE International Journal of Commercial Vehicles* (2018)

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 M. 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 optimized them for solar-cell device fabrication and testing. These solar cells afforded photovoltaic outputs that were comparable to those of the industrial standard. These results have been published in *Advanced Energy Materials*, showcasing the power of data-driven materials discovery.

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.

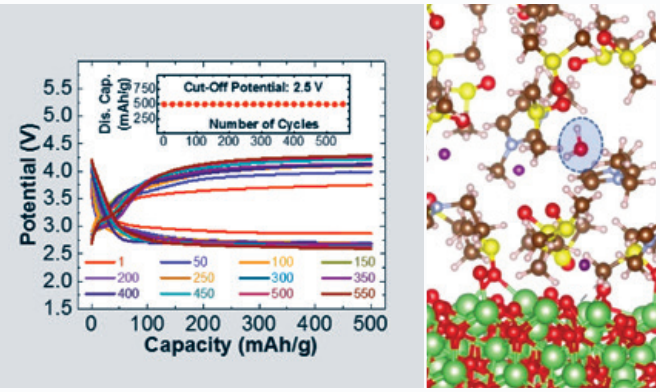
Cooper, C. B., E. J. Beard, Á. Vázquez-Mayagoitia, L. Stan, G. B. G. Stenning, D. W. Nye, J. A. Vigil, T. Tomar, J. Jia, G. B. Bodedla, S. Chen, L. Gallego, S. Franco, A. Carella, K. R. J. Thomas, S. Xue, X. Zhu, and J. M. Cole. "Design-to-Device Approach Affords Panchromatic Co-Sensitized Solar Cells," *Advanced Energy Materials* (December 2018), John Wiley and Sons.

Materials Science

Lithium-Oxygen Battery with Long Cycle Life in a Realistic Air Atmosphere

PI Larry Curtiss
INST Argonne National Laboratory
HOURS DD, 20 Million Core-Hours

A B



(A) Voltage profiles for a Li-O_2 cell based on a MoS_2 cathode, ionic liquid/dimethyl sulfoxide electrolyte and lithium carbonate coated lithium anode with a cycle life of over 500 cycles in air. **(B)** Results of an *ab initio* molecular dynamics simulation using VASP of the electrolyte used in the Li-O_2 cell that helped explain its stability. *Image: Mohammad Asadi, et al.,* Nature

Previous experimental designs of Li-O_2 batteries have failed to operate in a true natural air environment due to the oxidation of lithium anodes by air components and to the production of undesirable byproducts on cathodes (a result of combining lithium ions with carbon dioxide and water vapor). These byproducts gum up the cathodes, which eventually become completely coated and nonfunctional during charge and discharge cycles. To circumvent this problem, these batteries have often relied on tanks of pure oxygen, which severely limits their practicality.

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

Using molecular dynamics simulations made possible by ALCF supercomputers , the team overcame these challenges by uniquely combining the three main components of any battery—anode, cathode, and electrolyte—to prevent anode oxidation and the buildup of battery-killing byproducts on the cathode, which permitted operation in a natural air environment. The researchers coated the lithium anode with a thin layer of lithium carbonate that selectively allowed the passage of lithium ions and prevented unwanted air components, such as nitrogen, from reaching the anode. The cathode employed a lattice structure with a molybdenum disulfide catalyst and a novel hybrid electrolyte made of ionic liquid and dimethyl sulfoxide that helped facilitate Li-O_2 reactions, minimize reactions with ambient elements, and boosted the battery's efficiency. The complete architectural overhaul of the battery involved redesigning its every part to enable desirable reactions and block those that would kill the battery.

RESULTS

In a study published in *Nature*, the researchers reported a new design for a Li-O_2 battery cell that operates by reacting with air over numerous charge and discharge cycles. The battery was still functioning after a record-breaking 700 such cycles, which, being the first demonstration of a true Li-O_2 design, represents a significant advancement.

IMPACT

The new Li-O_2 cell architecture is a promising step toward engineering the next generation of lithium batteries with much higher specific energy density than lithium-ion batteries.

PUBLICATIONS

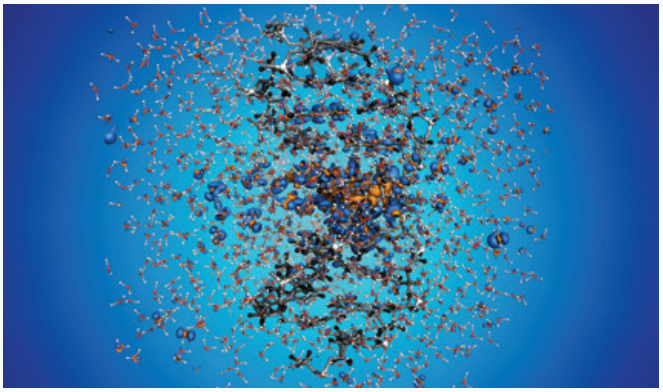
Asadi, M., B. Sayahpour, P. Abbasi, A. T. Ngo, K. Karis, J. R. Jokisaari, C. Liu, B. Narayanan, M. Gerard, P. Yasaei, X. Hu, A. Mukherjee, K. C. Lau, R.S. Assary, F. Khalili-Araghi, R. F. Klie, L. A. Curtiss, and A. Salehi-Khojin. "A Lithium-Oxygen Battery with a Long Cycle Life in an Air-like Atmosphere," *Nature* (March 2018), Springer Nature.

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 and DNA 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 quantum-mechanical excitation of electrons; however, recent innovations in first-principles calculation methodologies and massively parallel supercomputers have enabled accurate simulations of these processes at the atomistic level. 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 and understand the role of the (semi-)core electrons when matters are exposed to ion radiations beyond the typical proton radiation.

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 predominantly excite core electrons.

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.

PUBLICATIONS

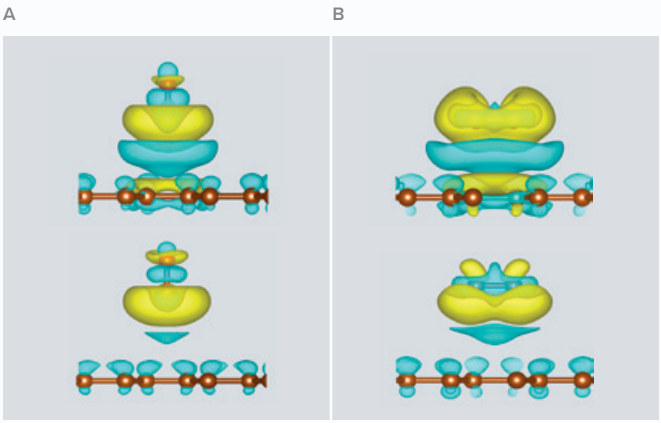
Lee, W.-C. and A. Schleife. "Electronic Stopping and Proton Dynamics in InP, GaP, and $In_{0.5}Ga_{0.5}P$ from First Principles," *European Physical Journal B* (October 2018), Springer.

Lee, W.-C. and A. Schleife. "Novel Diffusion Mechanism in the Presence of Excited Electrons: Ultrafast Electron-Ion Dynamics in Proton-Irradiated Magnesium Oxide," *Materials Today* (October 2018), Elsevier.

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 (O_2), 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 (DFTs): 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 O_2 molecules on graphene surfaces.

RESULTS

Using simulations on Mira to examine various orientations of O_2 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.

PUBLICATIONS

Song, S., M.-C. Kim, E. Sim, A. Benali, O. Heinonen, and K. Burke. “Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes,” *Journal of Chemical Theory and Computation* (April 2018), American Chemical Society.

Shin, H., A. Benali, Y. Luo, E. Crabb, A. Lopez-Bezanilla, L. E. Ratcliff, A. M. Jokisaari, and O. Heinonen. “Zirconia and Hafnia Polymorphs: Ground-State Structural Properties from Diffusion Monte Carlo,” *Physical Review Materials* (July 2018), American Physical Society.

Benali, A., Y. Luo, H. Shin, D. Pahls, and O. Heinonen. “Quantum Monte Carlo Calculations of Catalytic Energy Barriers in a Metallorganic Framework with Transition-Metal-Functionalized Nodes,” The Journal of Physical Chemistry C (June 2018), American Physical Society.

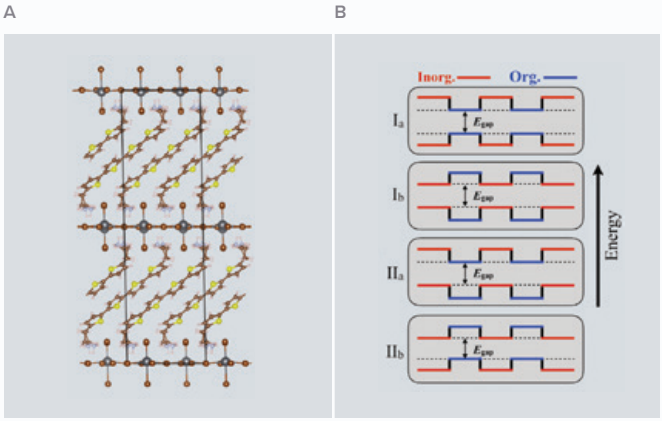
Luo, Y., K. P. Esler, P. R. C. Kent, and L. Shulenburger. “An Efficient Hybrid Orbital Representation for Quantum Monte Carlo Calculations,” *The Journal of Chemical Physics* (August 2018), American Institute of Physics.

Materials Science

Understanding Electronic Properties of Layered Perovskites with Extreme-Scale Computing

PI Volker Blum
INST Duke University

HOURS Theta ESP, 10 Million Core-Hours



(A) The supercell structure of a prototypical layered hybrid perovskite. Planar layers represent inorganic structures, while organic chains are ordered in diagonal arrangements. **(B)** Possible energy level schemes for an alternating organic-inorganic perovskite are shown with the overall band gap indicated by arrows and dashed lines. *Image: Chi Liu and Volker Blum, Duke University*

As with the flow of water, that of electrons can produce useful outcomes. It is therefore important to control the energy levels and flow of electrons and their counterparts, so-called holes, in high-quality electronic materials. One class of such materials are layered hybrid organic-inorganic perovskites (HOIPs), well-organized structures that combine organic and inorganic components (e.g., chains of doubly bonded molecular rings and ionic layers, respectively) to manipulate electron flow and the resulting light emission or absorption. Using ALCF supercomputing resources, Duke University researchers have demonstrated the possibility of understanding HOIPs as analogous to a system of "electron" and "hole" containers; this work could help create new materials with tunable optical properties.

CHALLENGE

HOIPs are semiconductor materials with opto-electronic properties for the production or capture of light. Laboratory experiments on synthesized HOIPs suggest perovskites could be designed with tailored properties, but the combinatorial nature of exploring potential materials presents significant obstacles (empirical models, meanwhile, demand more complex results and/or studies for validation). The researchers worked to show how the electronic properties of HOIPs can be quantitatively predicted by computation and systematically adjusted by separately modifying the organic and inorganic components, and, furthermore, how a quantum-well model can describe these properties.

APPROACH

Empirical models suggested that the interfaces created by layering hybrid perovskites would give rise to an electronic structure that formed quantum wells, which could be staggered to produce and transport an array of electron carriers in the presence of light. High-accuracy, all-electron calculations were carried out for confirmation, made possible through the employment of an efficient eigensolver and by scaling the density-functional code FHI-aims for use on the massively parallel Theta machine.

The contributions of ALCF staff included helping to port the FHI-aims code and optimize functions on Theta to enable large-scale linear algebra computations.

RESULTS

Calculations were particularly needed to separately adjust the nature of organic and inorganic layers. These calculations utilized experimental structures of a canonical 2D HOIP as starting points, providing insight into why one analog exhibited strong emission, whereas others were substantially quenched. Results were detailed in a paper published in *Physical Review Letters*.

IMPACT

There is a technological rush for materials with tunable optoelectronic properties, for which HOIPs are excellent candidates. In addition to impacting solar energy and optoelectronics research, this work benefits the computational physics and materials science communities by extending the capabilities of high-accuracy electronic materials simulations in general.

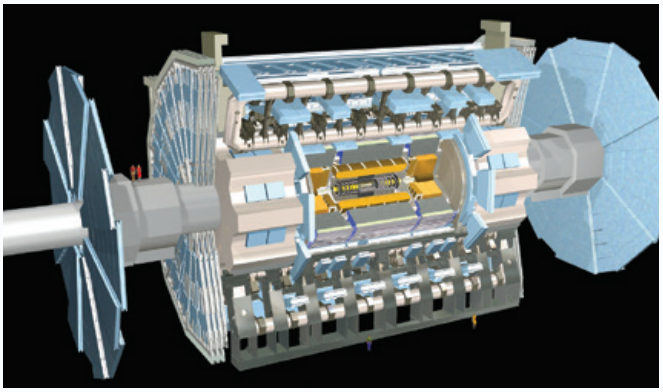
PUBLICATIONS

Liu, C., W. Huhn, K.-Z. Du, Á. Vazquez-Mayagoitia, D. Dirkes, W. You, Y. Kanai, D. B. Mitzi, and V. Blum. "Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites," *Physical Review Letters* (October 2018), American Physical Society.

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 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 were 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. This work was done in parallel and depended on software containerization given the different physics releases and libraries required for each step. Over 37 million events have been simulated on Theta, with many validating the workflow and chip architecture to ensure physics results produced agree with those from previous systems. The team's established functionality has permitted the generation of custom datasets that will be used to study machine learning techniques that could replace custom algorithms in the reconstruction.

IMPACT

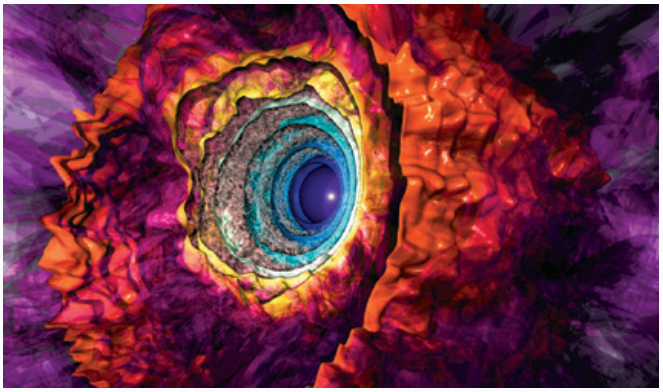
This project is increasing the scientific reach of LHC experiments to probe the fundamental forces and particles that make up the universe. High-precision measurements will be the driver of discovery in the next 10 years of LHC physics analyses, and ALCF computing resources will be essential for success. 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.

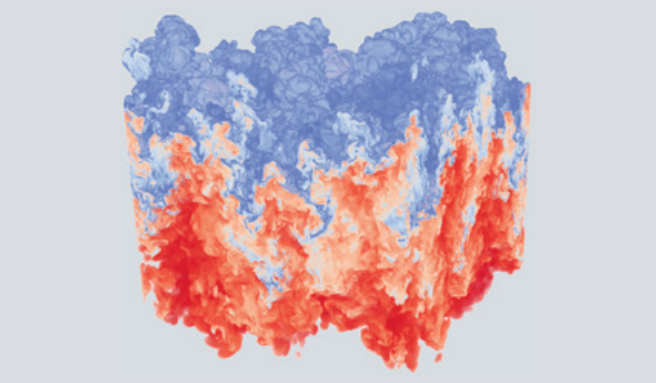
PUBLICATIONS

Jian, 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

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 at an unprecedented resolution of 1,024 x 1,024 x 2,048 grid points. *Image: Donxiao Zhao, University of Rochester*

The 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 (ICF) 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 ICF implosions.

CHALLENGE

RTI, which has hindered yields in ICF, 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 third of the Mira system (roughly 260,000 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 papers published in *Physical Review Letters*, *Physical Review E*, and *Physical Review Fluids*.

IMPACT

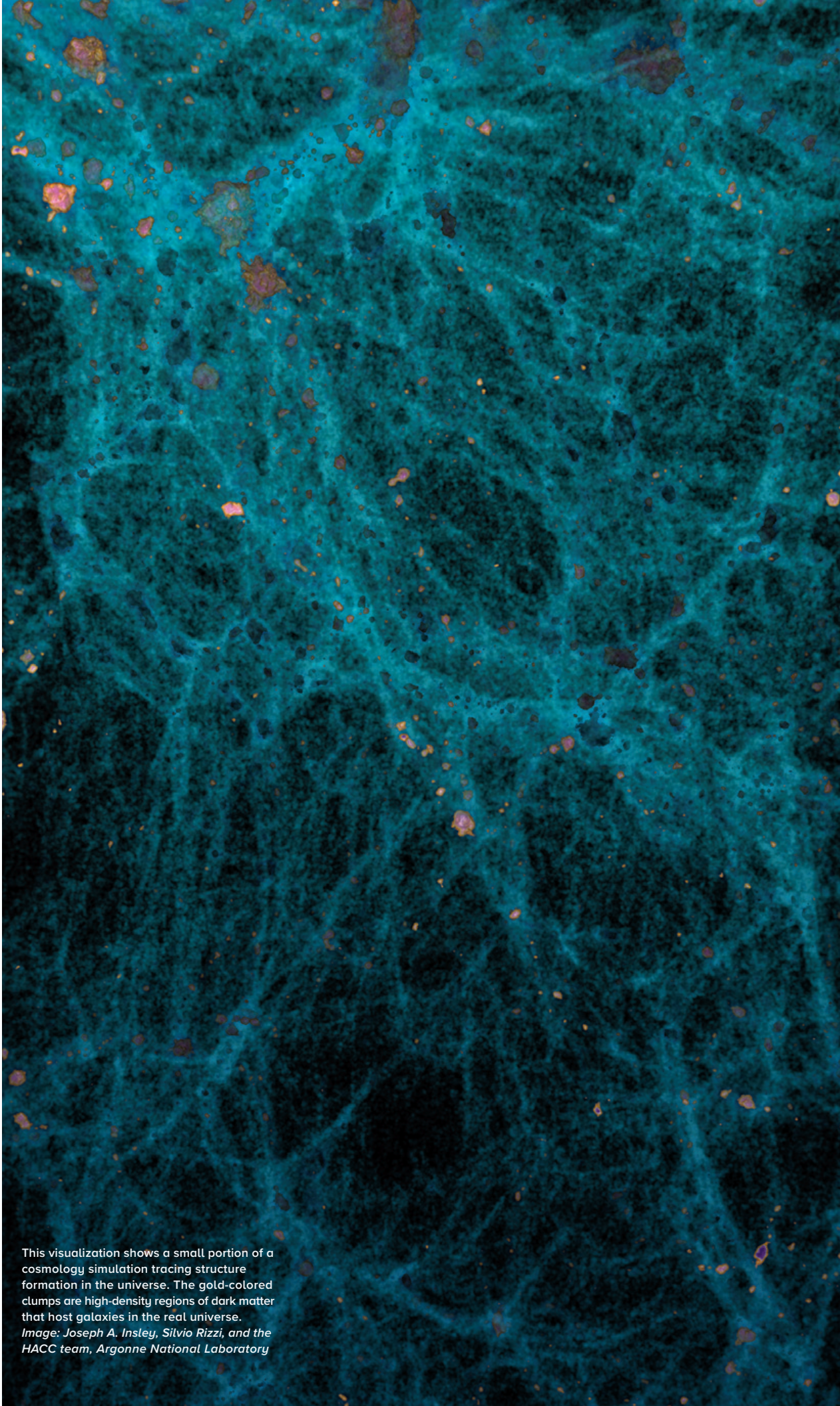
Beyond bringing nuclear fusion closer to realization as a viable and virtually limitless energy source, this work carries important ramifications for modeling implosion physics, astrophysics, oceanic flows, and combustion science.

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.

Zhao, D. and H. Aluie. "Inviscid Criterion for Decomposing Scales," *Physical Review Fluids* (May 2018), American Physical Society.

Zhang, H., R. Betti, R. Yan, D. Zhao, D. Shvarts, and H. Aluie. "Self-Similar Multimode Bubble-Front Evolution of the Ablative Rayleigh-Taylor Instability in Two and Three Dimensions," *Physical Review Letters* (October 2018), American Physical Society.



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.
Image: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory

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

2018–2019 ALCC Projects

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 SolarPowered 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 Projects

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

ALCF Publications

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

The publications are listed by their publication dates. An asterisk after a name indicates an ALCF author. ALCF publications are listed online at alcf.anl.gov/publications.

January

Aguilar, M., et al. (AMS collaboration). "Observation of New Properties of Secondary Cosmic Rays Lithium, Beryllium, and Boron by the Alpha Magnetic Spectrometer on the International Space Station," *Physical Review Letters* (January 2018), APS. doi:10.1103/PhysRevLett.120.021101.

Aktulga, H. M., C. Knight, P. Coffman, K. A. O'Hearn, T.-R. Shan, and W. Jiang. "Optimizing the Performance of Reactive Molecular Dynamics Simulations for Many-Core Architectures," *The International Journal of High Performance Computing Applications* (January 2018), SAGE Publications. doi:10.1177/1094342017746221.

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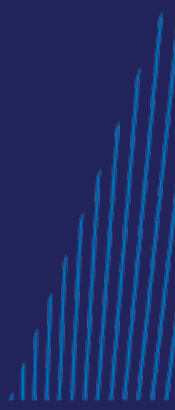

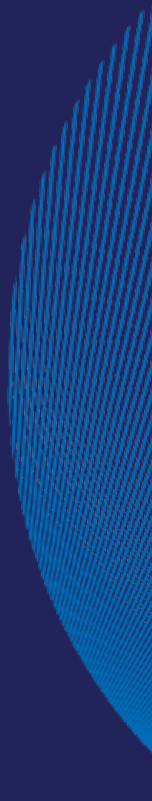

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