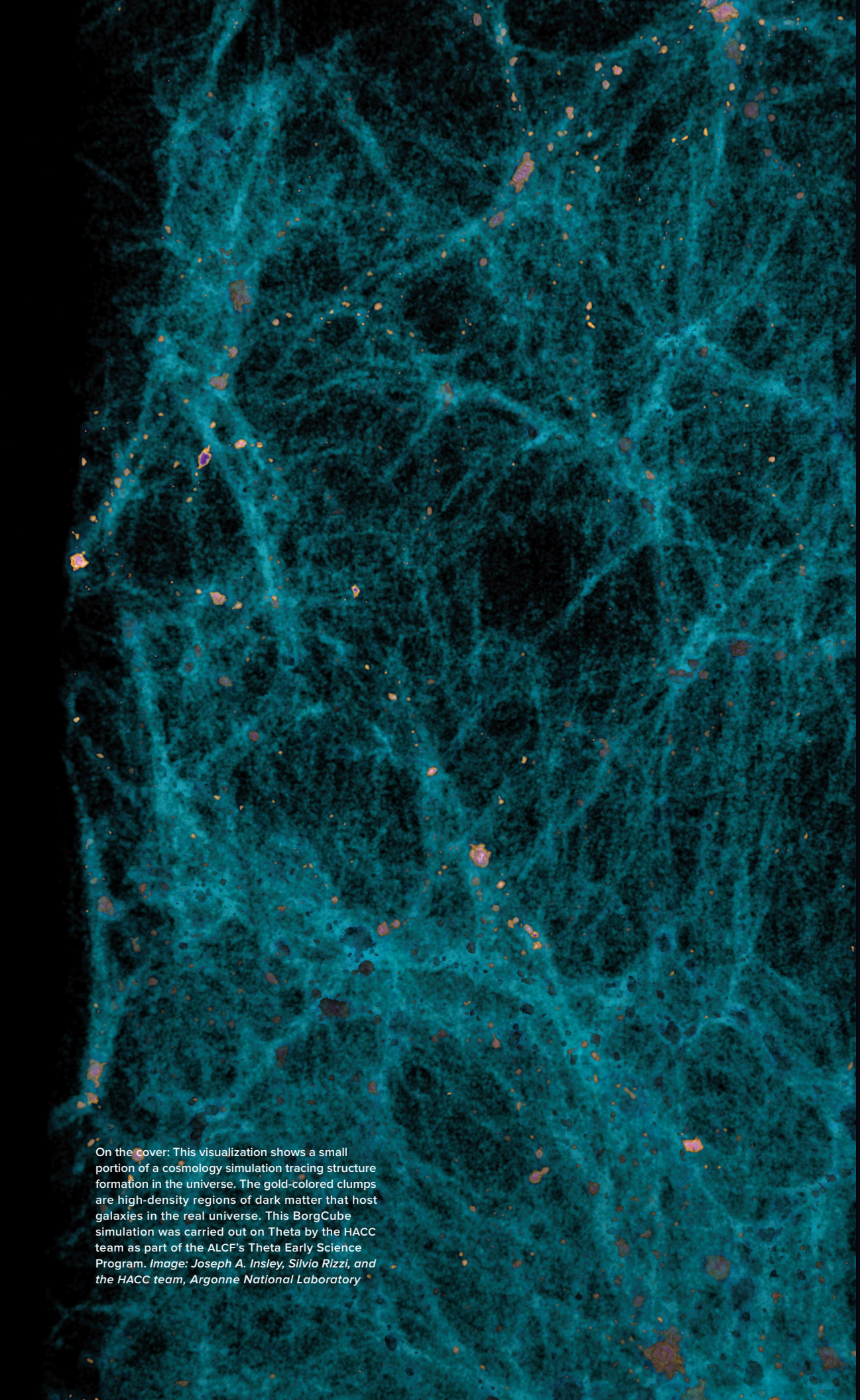
ARGONNE LEADERSHIP
COMPUTING FACILITY

Argonne
NATIONAL LABORATORY

2017

Annual Report



On the cover: 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. This BorgCube simulation was carried out on Theta by the HACC team as part of the ALCF's Theta Early Science Program. *Image: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory*

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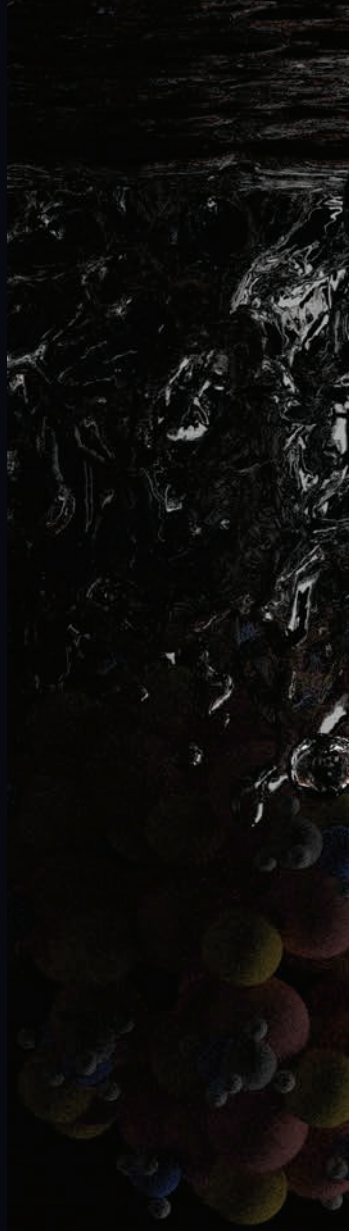
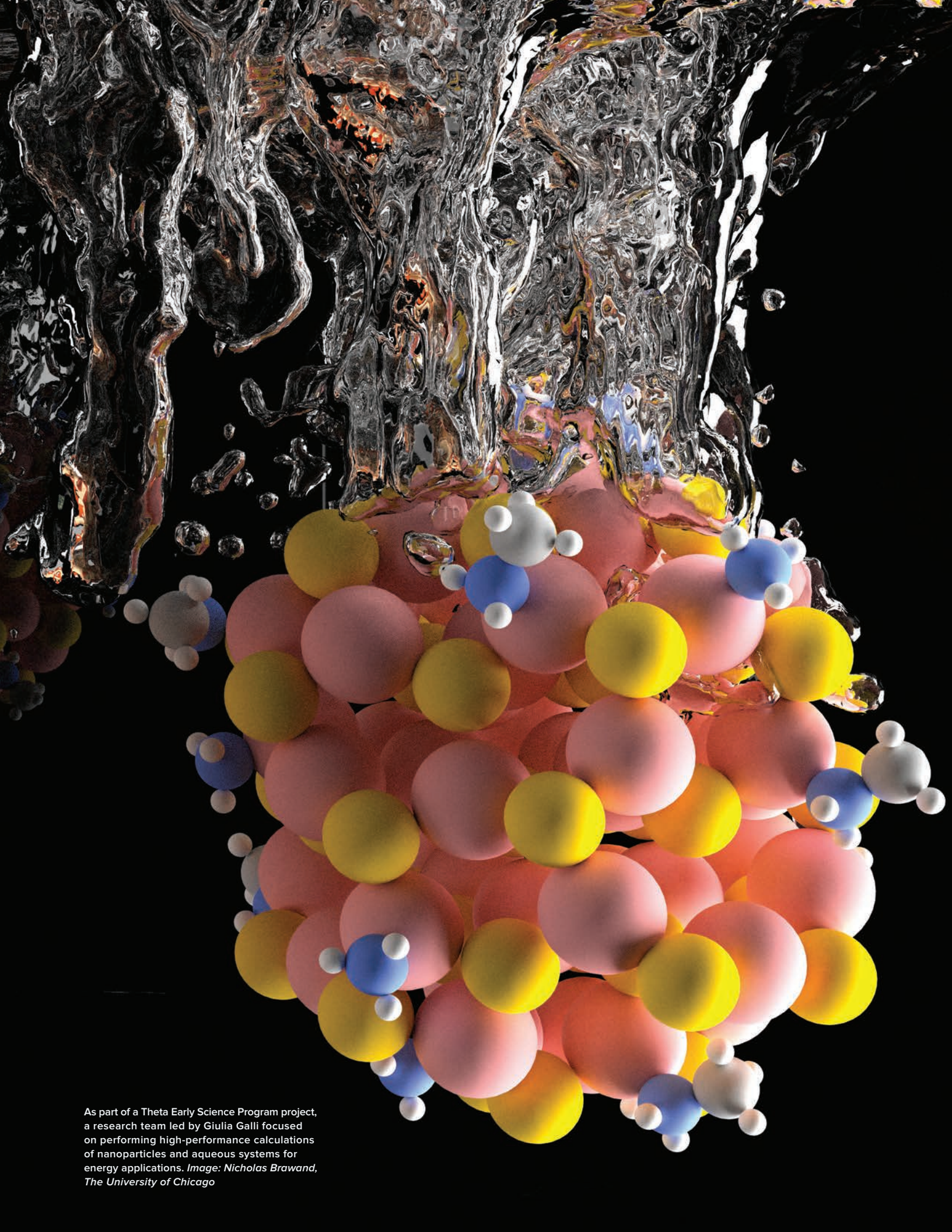
2017 Annual Report

YEAR IN REVIEW

The Argonne Leadership Computing Facility (ALCF) provides supercomputing resources and expertise to the research community to accelerate the pace of discovery and innovation in a broad range of science and engineering disciplines.





As part of a Theta Early Science Program project, a research team led by Giulia Galli focused on performing high-performance calculations of nanoparticles and aqueous systems for energy applications. *Image: Nicholas Brawand, The University of Chicago*

DIRECTOR'S MESSAGE

Michael E. Papka
ALCF Director

Operating leadership-class systems for the research community means operating at the edge of computing capabilities, while offering the greatest capacity for breakthrough science.

The ALCF performed its mission in 2017—launching a next-generation system, supporting a growing number of simulation and data science projects, and training future users—while making substantial progress toward new collaborations and new capabilities for new workloads.

The addition of the ALCF's latest supercomputer, Theta, doubled our capacity to do impactful science and marks the next waypoint in our journey to exascale computing. Notably, nearly all of the Theta Early Science projects reported significant science results, capping off another successful Early Science Program used to ready a new architecture for a diverse workload on day one.

The ALCF is now operating at the frontier of data centric and high-performance supercomputing, with powerful capabilities for equally supporting data, learning, and simulation projects. We will continue to bolster the data and learning programs alongside the simulation science program as we prepare for the ALCF's future exascale system, Aurora, expected in 2021. Our goal of science on day one, in all three areas, requires much work: Aurora will require not only innovation in parallel processing and network and storage performance, but also new software and tools to process the vast quantities of data needed to train deep learning networks to find patterns in data.

We are also adding new services that make our computing and data analysis capabilities available to scientific users working in far-flung places, such as large experiments and observatories. In 2017, ALCF staff deployed a pilot program to allow easier access to ALCF systems by giving external users the ability to inject jobs from outside the facility. Other possible future services include data transfer workflows and co-scheduling between ALCF systems.

I want to take a moment to recognize the many staff-directed training, outreach, and mentoring efforts, from the summer student research program to the Argonne Training Program on Extreme-Scale Computing to our many topical seminars and hands-on workshops that serve our users of today and prepare our users of tomorrow. This extends to the growing number of activities at Argonne's Joint Laboratory for Systems Evaluation as well, where ALCF researchers evaluate future HPC systems components and platforms.

This annual report offers readers a deep dive into the many activities happening at the ALCF. As the ALCF has done throughout its history, we remain dedicated to supporting our users' needs. It is a privilege to serve the science teams that use our resources to turn data into insights and competitive advantages. Most of all, I am deeply proud of the staff for what they do every day for our facility.

Operations and Science Updates

Operations

When Theta, our new Intel-Cray system, entered production mode in July, we began providing our user community with a new resource equipped with advanced capabilities for research involving simulation, data analytics, and machine learning techniques. Along with Mira and Cetus, we now operate three systems on the Top 500 list of the fastest supercomputers in the world. Our goal is to ensure that our supercomputers and all of the supporting resources that go along with them—computing clusters, storage systems, network infrastructure, systems environments, and software tools—are stable, secure, and highly available to users.

In 2017, our team worked tirelessly to integrate Theta into our supercomputing environment. Over the course of the year, we performed two upgrades on the system, bringing it to 24 racks, with 4,392 nodes and a peak performance of 11.69 petaflops.

We have also been heavily involved in preparations for our future exascale system, Aurora. This effort includes working closely with Intel and Cray to provide guidance on architectural features and the system's software stack. This collaborative work will only intensify as we work toward delivering Aurora in 2021.

In addition to working with the machines, we also interact directly with users, providing technical support to resolve issues as they arise. In 2017, we supported 1,000 allocations on five machines, on-boarded nearly 600 new users, and addressed more than 6,500 support tickets.

We also deployed two new services to support the evolving needs of our user community. Our Jupyter Notebook service provides staff members and users with a web-based tool that is great for supporting collaborative research, as well as teaching. HTCondor-CE, a gateway software service that enables remote job submission, makes it easier for large-scale collaborative projects, like CERN's Large Hadron Collider, to integrate ALCF computing resources into their workflows.

Finally, we developed a new web application for Director's Discretionary allocation requests. The new site allows us to better manage the request process by enabling staff members to easily filter and search for reviews, and check on the status of previous requests.

Mark Fahey
ALCF Director of Operations

Science

With Theta and Mira now operating alongside each other, we have two diverse petascale architectures to power scientific discoveries and engineering innovations.

To prepare Theta to deliver science on day one, our Early Science Program (ESP) gave research teams pre-production time on the system for science and code development projects. The program was a great success, with teams achieving both application performance improvements and science advances, while paving the way for the larger ALCF user community to run on the supercomputer.

In 2017, our users consumed more than 8 billion combined core-hours on our systems. Their research produced some impressive results, including publications in high-impact journals, such as *Science, Nature,* and *Physical Review Letters*. In total, our users published more than 200 papers this year.

In addition to delivering scientific achievements, ALCF users also made advances in computational methods, such as data mining and deep learning, demonstrating new tools to enable data-driven discoveries. Much of this research has been enabled by our ALCF Data Science Program (ADSP), which expanded from four to eight projects in 2017.

The use of emerging computational methods aligns with our paradigm shift—to support data and learning approaches alongside traditional simulation-based research. Together, these three areas of scientific computing provide a powerful new model for using leadership computing resources for science and discovery.

Next year, we plan to issue a call for proposals to expand our Aurora ESP to include 10 additional projects focused on data and learning. The new projects will complement the 10 simulation-based projects currently underway, providing a diverse set of projects that will help advance our simulation, data, and learning capabilities for exascale systems.

This brings us to Aurora, now slated to be the nation's first exascale system when it is delivered in 2021. In addition to our work to prepare applications and methods for exascale through ESP and ADSP, our researchers are evaluating new HPC trends, tools, and architectures to help set the stage for the future of the ALCF.

Katherine Riley
ALCF Director of Science

ALCF at a Glance

About ALCF

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

As a key player in the nation's efforts to deliver future exascale computing capabilities, the ALCF is also helping to shape a new paradigm for scientific computing—the convergence of simulation, data analytics, and machine learning.

ALCF computing resources are 10 to 100 times more powerful than systems typically used for scientific research and are available to researchers from academia, industry, and government agencies.

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

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

Core-hours of compute time

8B

Active projects*

356

Facility users*

976

Publications

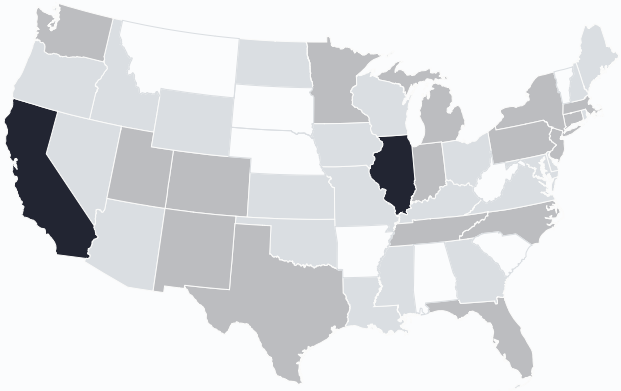
211

Supercomputers on the Top500 list

3

*Fiscal year 2017

2017 ALCF Users by State



100+ Users

California
Illinois

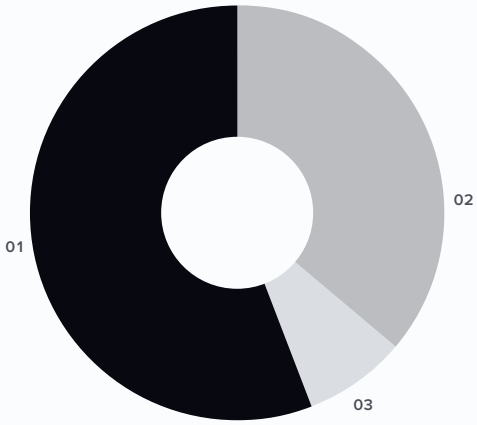
11–100 Users

Colorado
Connecticut
Florida
Indiana
Massachusetts
Michigan
Minnesota
New Jersey
New Mexico
New York
North Carolina
Pennsylvania
Tennessee
Texas
Utah
Washington

01–10 Users

Arizona
Georgia
Idaho
Iowa
Kansas
Kentucky
Louisiana
Maine
Maryland
Mississippi
Missouri
Nevada
New Hampshire
North Dakota
Ohio
Oklahoma
Oregon
Rhode Island
Virginia
Washington, D.C.
Wisconsin
Wyoming

2017 ALCF Users by Affiliation



01 Academia

545

02 Government

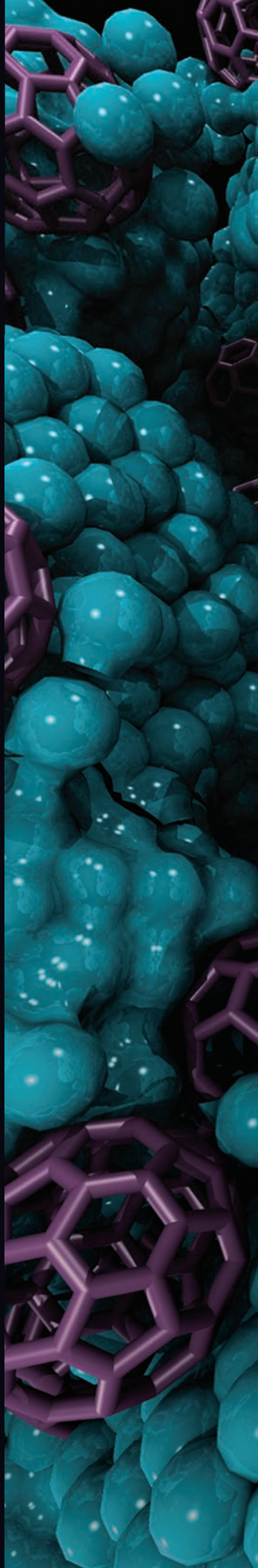
355

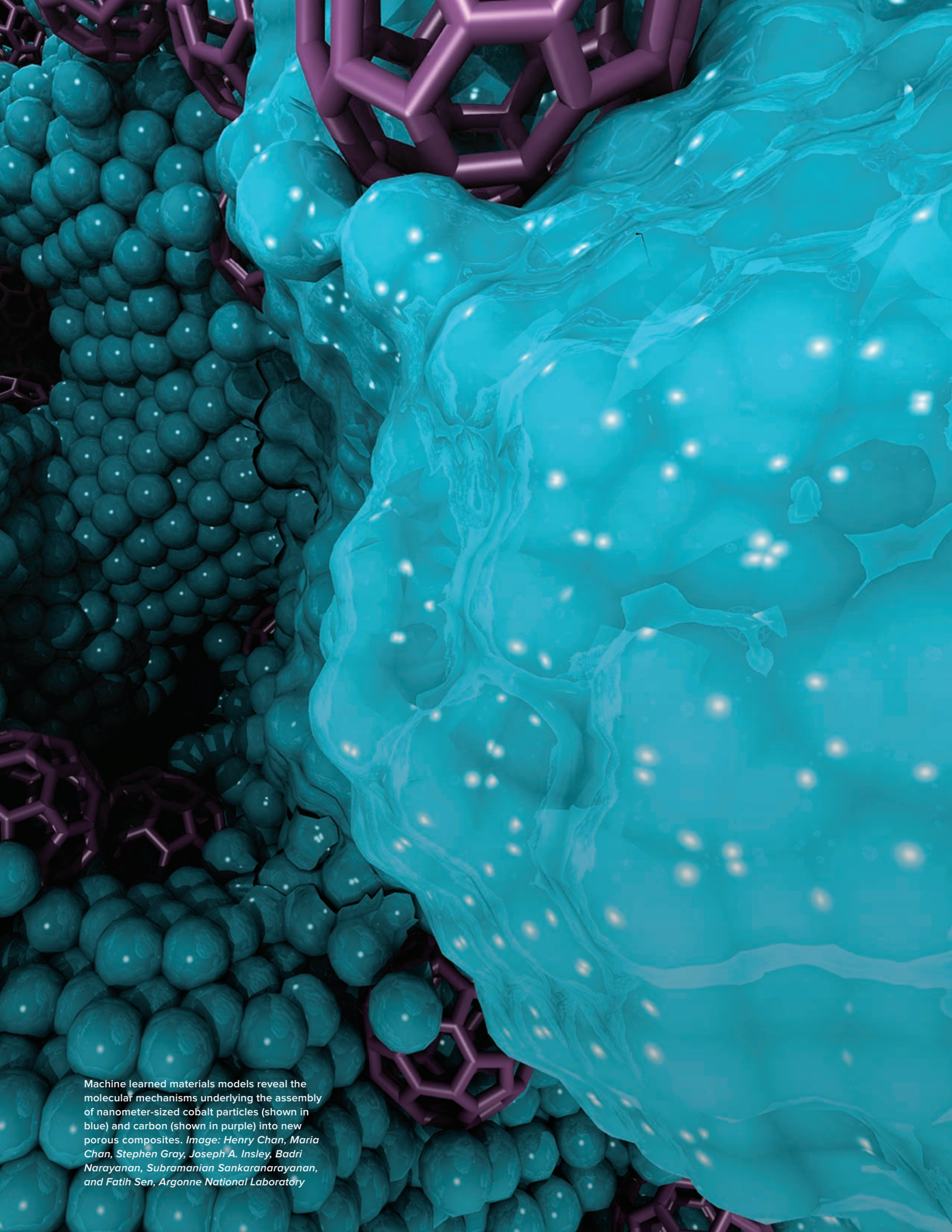
03 Industry

76

REDEFINING HPC

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





Machine learned materials models reveal the molecular mechanisms underlying the assembly of nanometer-sized cobalt particles (shown in blue) and carbon (shown in purple) into new porous composites. *Image: Henry Chan, Maria Chan, Stephen Gray, Joseph A. Insley, Badri Narayanan, Subramanian Sankaranarayanan, and Fatih Sen, Argonne National Laboratory*

The ALCF's New Paradigm: Simulation, Data, and Learning

To prepare for future exascale systems, the ALCF is expanding its scope beyond traditional simulation-based research to include data and learning approaches.

Simulation has long been the cornerstone of scientific computing. In the ALCF's first decade of operation, a majority of projects focused on using modeling and simulation to investigate the behavior of complex phenomena, ranging from combustion to biological systems.

While simulation-based research will remain a key component of the ALCF's workload, the facility is driving a new paradigm to expand the reach of its leadership computing resources by integrating data analysis and machine learning-based projects into the fold.

This new approach allows the ALCF to align with emerging research needs, while taking advantage of the innovative, new computing capabilities provided by Theta and the future exascale system, Aurora.

Data has always been an integral part of scientific computing, but the ever-growing amount of data being produced by large-scale simulations, telescopes, particle accelerators, and other experimental facilities calls for new analysis techniques.

Both data science (e.g., data analytics, data-intensive computing, advanced statistical analyses) and machine learning (e.g., deep learning, neural networks) provide methods that researchers can use to make sense of their increasingly complex and massive datasets.

Together, simulation, data, and learning will transform how ALCF supercomputers are used for scientific discovery and innovation.

For many projects, these computational approaches can be combined to create a feedback loop that helps scientists advance their studies.

For example, research teams can apply machine learning techniques to learn and make predictions from data generated by simulations. These findings can then be used to inform the development of improved models for subsequent simulations.

Ultimately, this integrated approach will help reduce simulation costs, increase data fidelity, and accelerate time to solution.

INCORPORATING DATA AND LEARNING RESEARCH

The ALCF started to make data and learning a priority in 2016, with the launch of the ALCF Data Science Program (ADSP). This new allocation program was created to support projects aimed at exploring and improving a variety of computational methods that could help enable data-driven discoveries across all scientific disciplines.

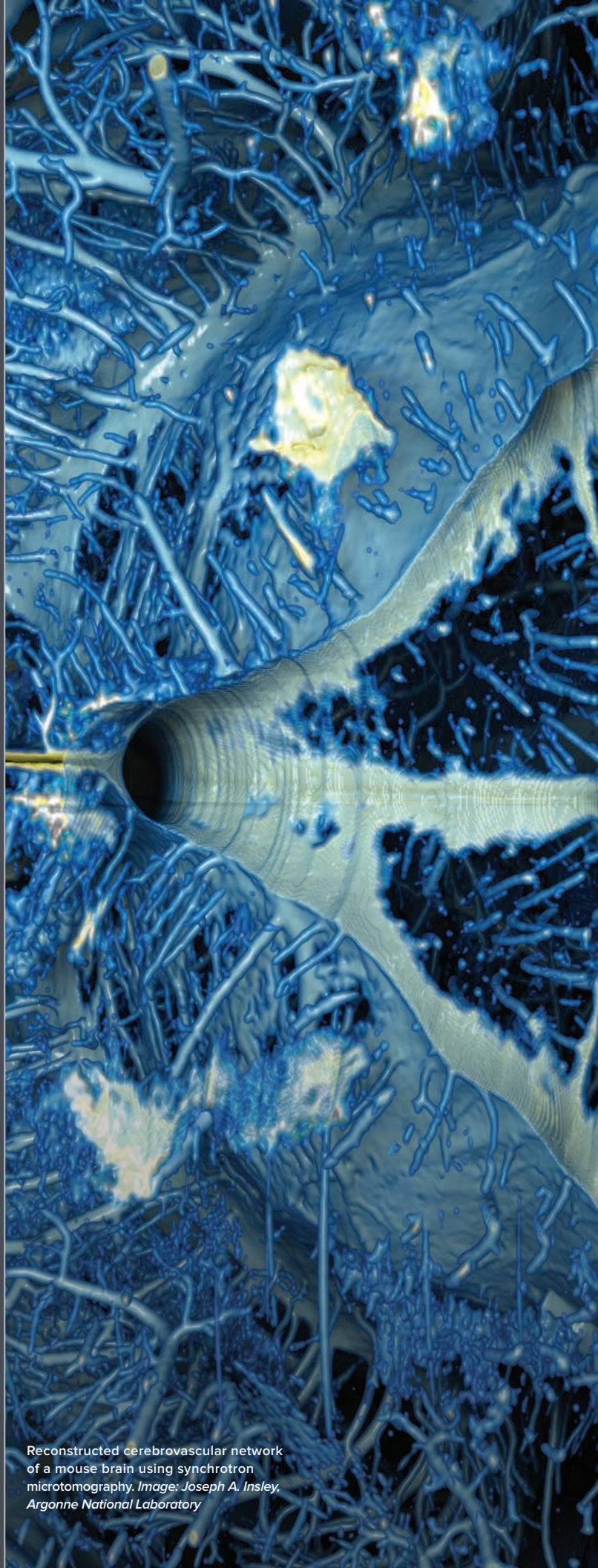
In its first two years, the ADSP has made great progress with several projects that integrate aspects of simulation, data, and learning.

For example, Jacqueline Cole, a scientist with a joint appointment at Argonne National Laboratory and the University of Cambridge, is developing a new material-by-design methodology. By using machine learning and data mining in conjunction with large-scale simulations and experiments, her project aims to identify new light-absorbing dye molecules for solar energy. The process involves building a large database of organic molecules that exhibit desirable structural and electronic qualities by data mining the properties of materials from 300,000 published research articles.

Another ADSP project, led by Rathakrishnan Bhaskaran of GE Global Research, is leveraging machine learning and large datasets generated by large-eddy simulations to develop data-driven turbulence models with improved predictive accuracy.

These are just a few of the unique crosscutting projects that illustrate how the convergence of simulation, data, and learning can be used to accelerate research.

In addition to the ADSP, the ALCF will expand its Aurora Early Science Program to include 10 new projects focused on data and learning in 2018.



Reconstructed cerebrovascular network of a mouse brain using synchrotron microtomography. *Image: Joseph A. Insley, Argonne National Laboratory*

Aurora: Argonne's Future Exascale Supercomputer

The ALCF's next-generation system, Aurora, is expected to be the nation's first exascale supercomputer when it is delivered in 2021.

The ALCF continues to prepare for the arrival of Aurora, a next-generation Intel-Cray system that will be capable of at least one exaflops, or one quintillion (10^{18}) calculations per second.

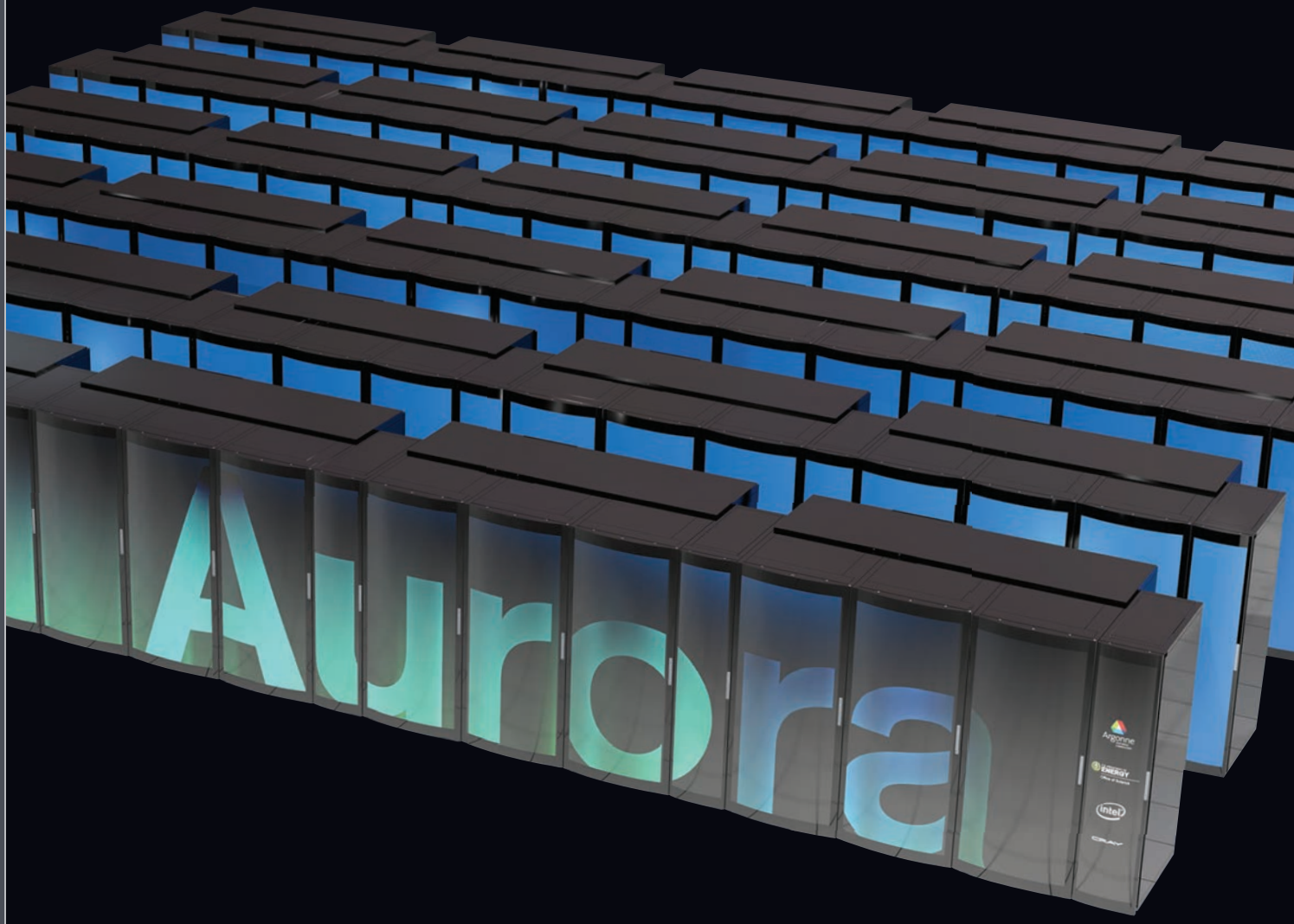
Slated to be the nation's first exascale system, the speed and scale of Aurora will be vastly greater than today's most powerful supercomputers.

The shift in plans for Aurora, which was initially scheduled to be a 180-petaflops supercomputer, is central to the ALCF's new paradigm for scientific computing—the expansion from traditional simulation-based research to include data and learning approaches.

With advanced capabilities for modeling and simulation, data science, and machine learning, Aurora's revolutionary hardware and software will power a new era of scientific discovery and innovation at the ALCF.

Expected Architectural Features

- More than 50,000 nodes
- Nodes will have high single-thread performance
- Nodes will enable exceptional performance with codes that have concurrency at a modest scale
- More than 5 petabytes of memory
- All memory will be high performance
- Memory in a node will be coherent
- Compute hardware will have equal access to all resources (memory, fabric, etc.)



Slated to be the nation's first exascale system when it is delivered in 2021, Aurora will help ensure continued U.S. leadership in high-end computing for scientific research.

Aurora Early Science Teams Prepare for Exascale

In 2017, the ALCF began its Aurora Early Science Program (ESP), with the selection of 10 projects to help prepare key applications for the architecture and scale of the next-generation system.

The current projects are serving as simulation-based projects. Next year, the ALCF will expand the program by issuing a call for proposals for 10 additional projects focused on data science and machine learning approaches.

The Aurora ESP provides science teams with dedicated time on Theta to carry out code development work and to conduct real science runs targeted at the future exascale supercomputer. The project teams attend training sessions and work closely with ALCF staff and vendors, Intel and Cray, to adapt their high-performance codes to Aurora's advanced architecture.

The teams also have access to training and hardware at the Oak Ridge Leadership Computing Facility (OLCF) and the National Energy Research Supercomputing Center (NERSC) to promote application code portability across heterogeneous architectures.

The following pages provide an overview of the 10 projects that got underway in 2017.

Simulation Projects

Benchmark Simulations of Shock-Variable Density Turbulence and Shock-Boundary Layer Interactions with Applications to Engineering Modeling

PI Sanjiva Lele, Stanford University

Design and Evaluation of High-Efficiency Boilers for Energy Production Using a Hierarchical V/UQ Approach

PI Martin Berzins, The University of Utah

Extending Moore's Law Computing with Quantum Monte Carlo

PI Anouar Benali, Argonne National Laboratory

Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann, Argonne National Laboratory

Extreme-Scale Unstructured Adaptive CFD

PI Kenneth Jansen, University of Colorado at Boulder

Free Energy Landscapes of Membrane Transport Proteins

PI Benoît Roux, The University of Chicago and Argonne National Laboratory

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang, Princeton Plasma Physics Laboratory

Lattice Quantum Chromodynamics Calculations for Particle and Nuclear Physics

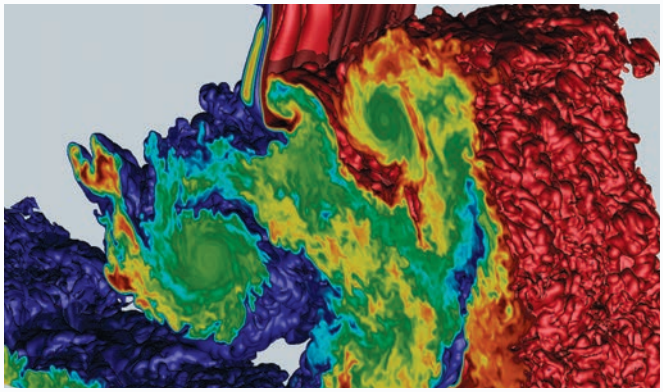
PI Paul Mackenzie, Fermilab

Metascalable Layered Materials Genome

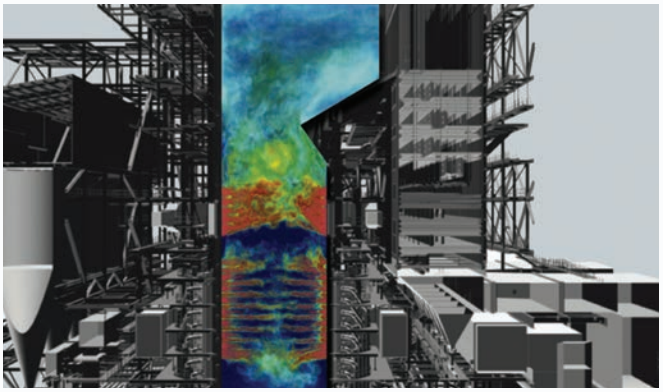
PI Aiichiro Nakano, University of Southern California

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

PI Thomas Dunning, Pacific Northwest National Laboratory



Simulation of shock interaction with a variable density inclined interface. *Image: Sanjiva Lele, Stanford University*



Large-eddy simulation prediction of instantaneous O_2 mass fraction in an ultra-supercritical coal boiler. *Image: Carbon-Capture Multidisciplinary Simulation Center, University of Utah*

Benchmark Simulations of Shock-Variable Density Turbulence and Shock-Boundary Layer Interactions with Applications to Engineering Modeling

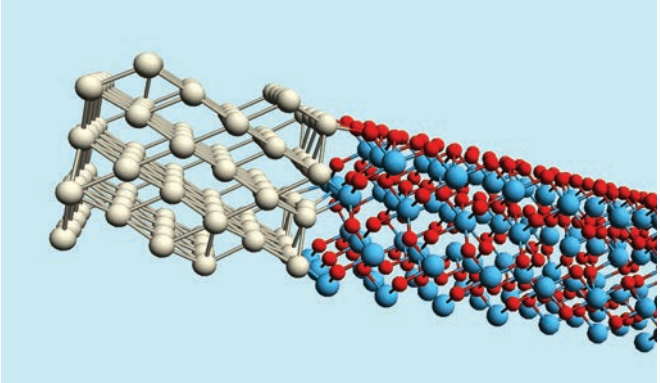
PI Sanjiva Lele
INST Stanford University
CODE SU2, PadeOps

Inertial confinement fusion and supersonic aircraft both involve the flow of gases in extreme conditions, including shock waves and turbulence. This project is focused on advancing scientific understanding of variable density turbulence and mixing, including shock interactions and near-wall effects. These phenomena apply to the interaction of the fuel capsule surface with the imploding plasma in inertial confinement fusion, and shock interaction with fuel streams in a supersonic jet engine as a way to improve combustion. In addition to providing a comprehensive assessment of shock-variable density turbulence interaction in a multifidelity setting, the ESP team plans to generate benchmark-quality datasets for validation and model development.

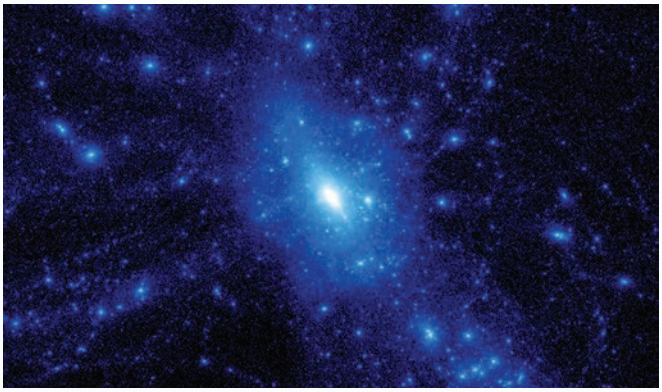
Design and Evaluation of High-Efficiency Boilers for Energy Production Using a Hierarchical V/UQ Approach

PI Martin Berzins
INST The University of Utah
CODE Uintah

This project aims to simulate and evaluate the design of a next-generation, ultra-supercritical coal boiler. The team plans to apply a novel computer science approach in conjunction with a hierarchical validation and uncertainty quantification (V/UQ) methodology to provide a simulation tool that can predict the thermal performance of the boiler with uncertainty bounds as constrained by observed data across multiple physical scales. The simulation data and resulting simulation tool have the potential to impact boiler design by minimizing capital investment, increasing boiler efficiency by 50 percent, and reducing CO_2 emissions by 50 percent.



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



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

Extending Moore's Law Computing with Quantum Monte Carlo

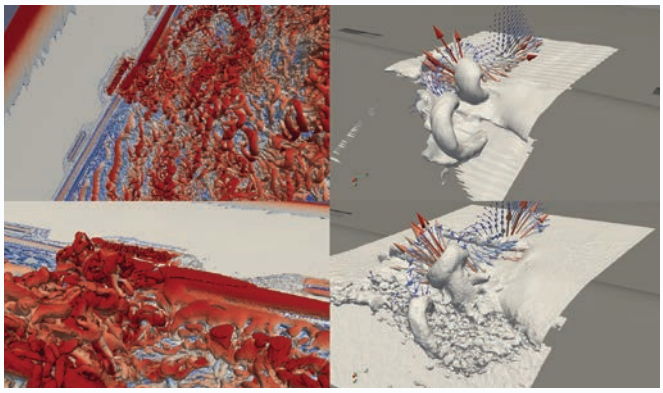
PI Anouar Benali
INST Argonne National Laboratory
CODE QMCPACK

For decades, massively parallel supercomputers have reaped the benefits—predicted by Moore's Law—of the relentless increase in density of components on chips, which also rapidly improved the performance of PCs and smartphones. This project aims to identify possible paths forward for extending Moore's Law in silicon complementary metal oxide semiconductor-based computing technologies. The researchers will tackle a fundamental materials problem impacting next-generation chips: electrical current leakage at the chip's interface with the widely used dielectric hafnium oxide. Simulating this problem with the highly accurate quantum Monte Carlo method is only now becoming computationally possible with supercomputers like Aurora.

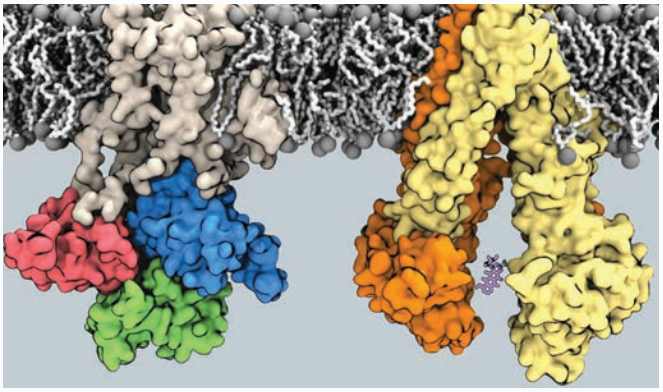
Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann
INST Argonne National Laboratory
CODE HACC

The analysis of observations from large-scale cosmological surveys requires extremely detailed simulations of structure formation in the universe. Building upon new capabilities recently implemented in the extreme-scale HACC code, this ESP project aims to carry out cosmological hydrodynamics simulations that cover the enormous length scales characteristic of large sky surveys, while at the same time capturing the relevant small-scale physics. The researchers will simulate large fractions of the universe, including not only gravity acting on dark matter, but also baryons (which make up visible matter such as stars) and gas dynamics using a new, smoothed particle hydrodynamics method. These simulations are deeply coupled with guiding and interpreting observations from present and near-future cosmological surveys.



This project will use Aurora to perform flow simulations of unprecedented scale and complexity. *Image: Kenneth Jansen, University of Colorado Boulder*



Membrane bound structures for the two transporter proteins to be investigated with this project. *Image: Jing Li and Huan Rui, the University of Chicago*

Extreme-Scale Unstructured Adaptive CFD

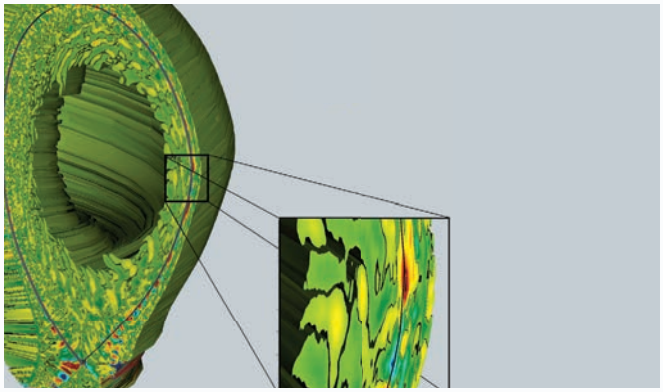
PI Kenneth Jansen
INST University of Colorado Boulder
CODE PHASTA

This project seeks to advance simulations in two complex flow regimes; aerodynamic flow control and multiphase flow. The aerodynamic flow control task involves performing simulations of an aircraft's vertical tail rudder at realistic flight conditions, while the multiphase flow task aims to simulate bubbly flows within realistic nuclear reactor geometries at an unprecedented scale. Both types of simulations will exploit anisotropic adaptive unstructured grids to match mesh length scales precisely to solution requirements, which will enable dramatic advances in computational modeling. The simulations will help inform the design of next-generation aircraft and nuclear reactors by providing insights into three-dimensional active flow control at flight scale and reactor heat exchanger flow physics.

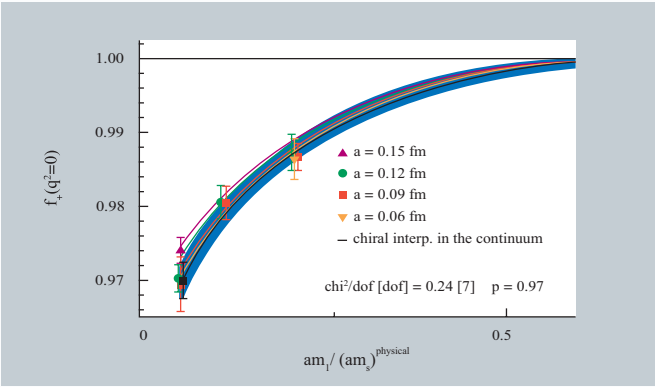
Free Energy Landscapes of Membrane Transport Proteins

PI Benoît Roux
INST The University of Chicago and Argonne National Laboratory
CODE NAMD

Membrane transport proteins play key roles in cellular biology functions. This includes natural processes as well as drug delivery and drug resistance. With this ESP project, researchers aim to use Aurora to provide an atomistic picture of how these proteins carry out their functions. The team will perform large-scale molecular dynamics simulations to determine the free energy landscapes underlying the function of two large membrane transporters. This work involves using advanced computational models to provide both detailed visualizations of large protein motions and quantitative predictions of the energetics of these processes.



Electrostatic tokamak edge turbulence from XGC simulation.
Image: Dave Pugmire, Oak Ridge National Laboratory



The form factor for the decay of a kaon into a pion and two leptons.
Image: Fermilab Lattice and MILC Collaborations

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

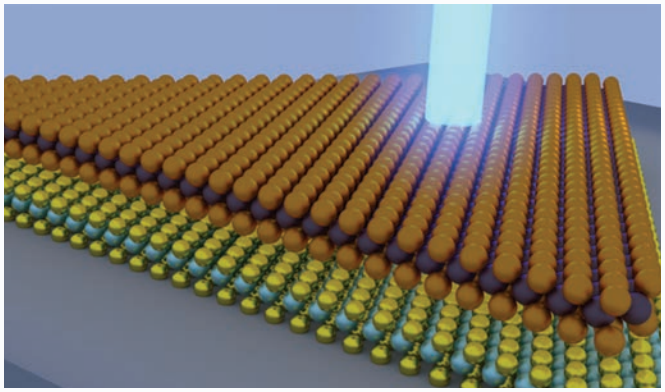
PI C.S. Chang
INST Princeton Plasma Physics Laboratory
CODE XGC

The behavior of plasma at the outer edge of a tokamak fusion reactor is critically important to the success of future fusion reactors such as ITER, now under construction in France. This ESP project aims to enhance the predictability of ITER performance, with a focus on the edge region, which is crucial for the confinement of burning plasma and a tolerable spread of heat on the reactor's wall surface. The team will use the XGC particle-in-cell code to simulate the multiscale behaviors of edge plasma in complex geometries. By advancing the understanding and prediction of plasma confinement at the edge, the team's research will help guide future experimental parameters and accelerate efforts to achieve fusion energy production.

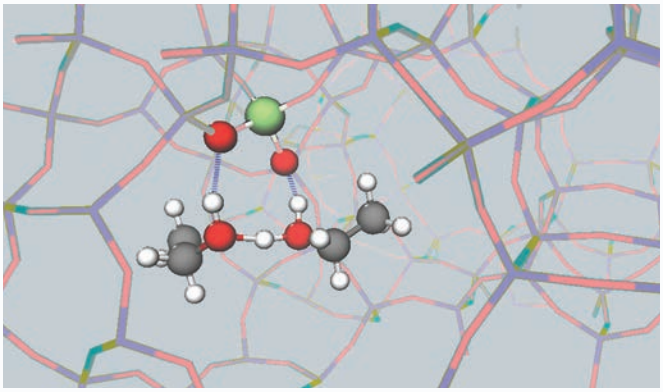
Lattice Quantum Chromodynamics Calculations for Particle and Nuclear Physics

PI Paul Mackenzie
INST Fermilab
CODE USQCD codes

This project will deliver lattice quantum chromodynamics (QCD) calculations that will have a major impact on high energy and nuclear physics research, offering critical support to the experimental programs in both areas. Lattice calculations are required to extract the fundamental parameters of the Standard Model (such as quark masses) from experiment. Evidence of physics beyond the Standard Model can be discovered if discrepancies are found between different methods for determining these parameters. The ESP team aims to perform several lattice QCD calculations on Aurora that are not possible on today's most powerful supercomputers.



This project will study photo-excitation dynamics in a stack of different transition metal dichalcogenide monolayers. *Image: Aravind Krishnamoorthy, University of Southern California*



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

Metascalable Layered Materials Genome

PI Aiichiro Nakano
INST University of Southern California
CODE NAQMD, RMD

With outstanding electronic, optical, magnetic, and chemical properties, functional layered materials are a promising area of research for many applications, including batteries, catalysts, and solar cells. For this ESP project, researchers will use Aurora to perform massive quantum mechanical and reactive molecular dynamics simulations aimed at advancing the computational synthesis and characterization of layered materials. The team's simulations, which will be validated by free-electron X-ray laser experiments, will provide much-needed information on the function-property-structure relationships of novel layered materials. Ultimately, this research will help guide the synthesis of new materials engineered for targeted applications.

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

PI Thomas Dunning
INST Pacific Northwest National Laboratory
CODE NWChemEx

This project seeks to develop a next-generation molecular modeling package that supports a broad range of chemistry research on a broad range of computing systems. In addition to improving code performance for exascale systems, the researchers will incorporate new computational approaches to dramatically reduce the cost of molecular simulations. The team's science campaign will address two challenges involved in the development of advanced biofuels: the design of feedstock for the efficient production of biomass; and the design of new catalysts for converting biomass-derived chemicals into fuels. The NWChemEx code will also be capable of addressing molecular challenges for many other energy-related applications, including batteries, combustion, and solar energy.

Theta: A New Architecture for Simulation, Data, and Learning

Now in production, the ALCF's new supercomputer is helping researchers pursue breakthroughs in a wide range of computational science and engineering projects.

Theta, the ALCF's new Intel-Cray supercomputer, entered production mode on July 1, 2017. The system now operates alongside Mira, an IBM Blue Gene/Q supercomputer, giving the ALCF two of the most powerful supercomputers in the world for open science.

Designed in collaboration with Intel and Cray, Theta is an 11.69-petaflops system equipped with Intel processors and interconnect technology, a novel memory architecture, a Lustre-based parallel file system, and Cray's HPC software stack.

In addition to providing advanced modeling and simulation capabilities, Theta's unique architectural features also support data-driven and machine-learning approaches, which are becoming increasingly significant drivers of large-scale scientific computing.

The system's innovative architecture is already enabling researchers to break new ground in scientific investigations that range from modeling the inner workings of the brain to developing new materials for renewable energy applications.

Upon entering production mode, Theta immediately began supporting several 2017–2018 ALCC projects, as well as projects from the ALCF Data Science Program. In 2018, the system will become available to researchers awarded computing time through the INCITE program.

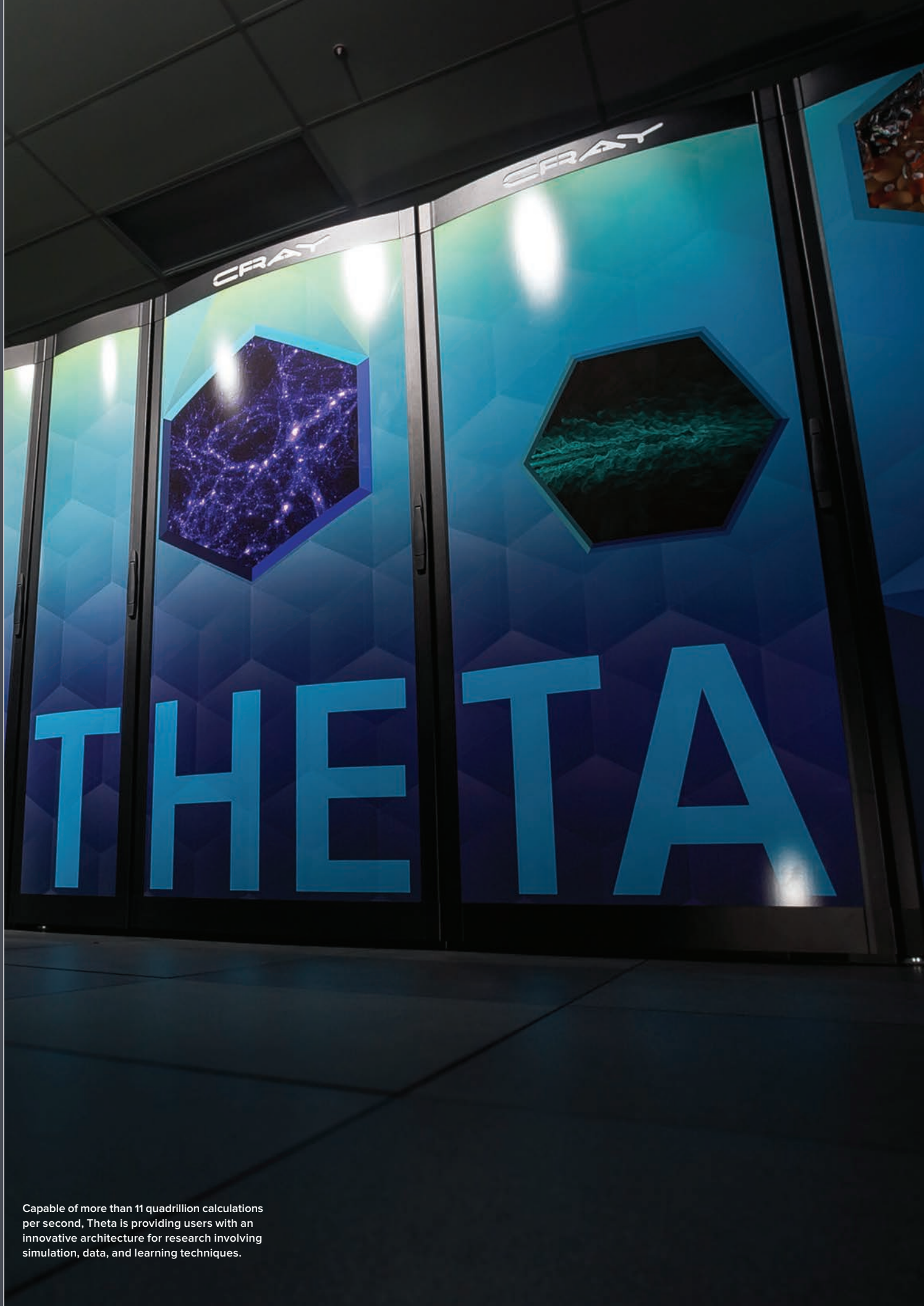
Theta Configuration

- 24 racks
- 4,392 nodes
- 281,088 cores
- 70.27 TB MCDRAM
- 843.26 TB DDR4
- 562.17 TB SSD
- Aries interconnect with Dragonfly configuration
- 10 PB Lustre file system
- Peak performance of 11.69 petaflops

Powering Science

Theta has several features that allow scientific codes to achieve high performance, including:

- High-bandwidth MCDRAM (300-450 GB/s depending on memory and cluster mode), with many applications running entirely in MCDRAM or using it effectively with DDR4 RAM
- Improved single-thread performance
- Improved vectorization with AVX–512
- Large total memory per node



Capable of more than 11 quadrillion calculations per second, Theta is providing users with an innovative architecture for research involving simulation, data, and learning techniques.

Preparing Theta for Science on Day One

Researchers participating in the Theta Early Science Program (ESP) achieved some notable technical and scientific advances, while paving the way for other users to run their applications on the ALCF's new supercomputer.

Modeled after the highly successful Mira ESP, the Theta program was conducted to prepare scientific applications for the architecture and scale of the facility's new Intel-Cray supercomputer.

Launched in 2015, the Theta ESP awarded computing time and resources to six science projects and six code development projects that would help ready the machine to deliver science on day one.

By bringing together computational scientists, code developers, and computing hardware experts, the Theta ESP created a collaborative environment for optimizing applications, characterizing the behavior of new hardware and software features, and solidifying libraries and infrastructure for future Theta users.

Even before Theta was installed at Argonne, the ESP teams, in collaboration with ALCF and vendor staff, began working diligently to adapt their applications for the system's new Intel-Cray architecture. The science teams were then able to use the critical pre-production time period (between system installation and full production) to pursue innovative computational science calculations.

The teams' efforts yielded notable successes in code modifications, algorithmic developments, and, in some cases, scientific advances. The following pages highlight the achievements of several of the Theta ESP projects.

Tier 1 Science Projects

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

PI Alexei Khokhlov, The University of Chicago

First-Principles Simulations of Functional Materials for Energy Conversion

PI Giulia Galli, The University of Chicago and Argonne National Laboratory

Free Energy Landscapes of Membrane Transport Proteins

PI Benoit Roux, The University of Chicago and Argonne National Laboratory

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

PI Fabien Delalondre, Ecole Federale Polytechnique de Lausanne

Next-Generation Cosmology Simulations with HACC: Challenges from Baryons

PI Katrin Heitmann, Argonne National Laboratory

Scale-Resolving Simulations of Wind Turbines with SU2

PI Juan Alonso, Stanford University

Tier 2 Code Development Projects

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

PI Mark Gordon, Iowa State University

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

PI Volker Blum, Duke University
Noa Marom, Carnegie Mellon University

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

PI Kenneth Jansen, University of Colorado Boulder

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

PI Christos Frouzakis, ETH Zurich

The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon

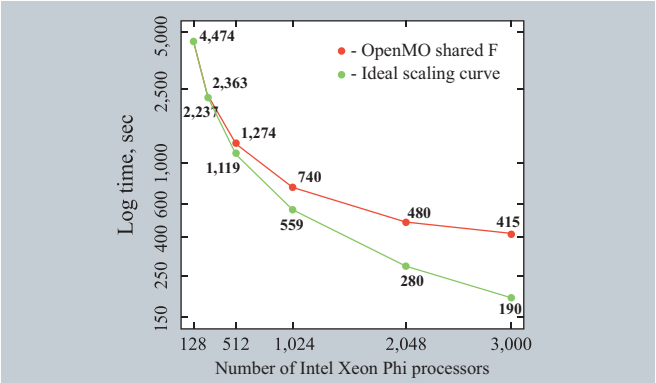
PI Paul Mackenzie, Fermilab

Quantum Monte Carlo Calculations in Nuclear Theory

PI Steven Pieper, Argonne National Laboratory

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

PI Mark Gordon
INST Iowa State University
CODE GAMESS



Scalability of the shared Fock MPI/OpenMP algorithm on Theta for the 5.0-nm benchmark system. *Image: Yuri Alexeev, Argonne National Laboratory; Michael D'mello, Intel; Mark Gordon and Kristopher Keipert, Iowa State University; Vladimir Mironov, Lomonosov Moscow State University; Alexander Moskovsky, RSC Technologies*

Graphene sheets are of interest to researchers for use in microlubricants. Researchers from Iowa State University, the Worcester Polytechnic Institute, and Argonne National Laboratory used graphene sheet simulations for benchmarking to optimize the GAMESS code on Theta. The team implemented two hybrid MPI/OpenMP Hartree-Fock (HF) algorithms in GAMESS, reducing the memory footprint by up to 200 times and the time to solution by up to six times on Theta's Knights Landing (KNL) architecture and Intel Xeon processors compared with the legacy code. These performance improvements will support future studies of graphene sheets and other research efforts using the GAMESS code.

The HF method is used to iteratively solve the electronic Schrödinger equation for a many-body system. Researchers use the resulting electronic energy and electronic wave functions to compute equilibrium geometries and characterize a variety of molecular properties. The HF solution represents a starting point for a wide range of higher-accuracy methods. The original MPI-based GAMESS HF implementation exhibits a very high memory footprint, because a number of its data structures are replicated across MPI ranks. For architectures with many cores such as Theta's KNL, the memory footprint of these data structures severely limits the size of the chemical systems that can fit within the system's memory.

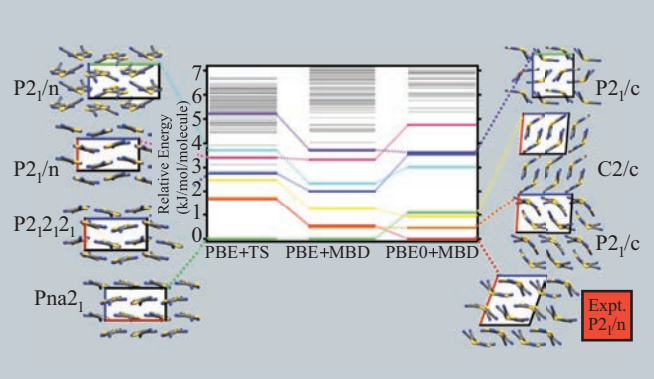
The ESP team optimized the HF implementation in the GAMESS electronic structure package for Theta's KNL architecture, implementing two new hybrid MPI/OpenMP HF algorithms that reduced the HF memory footprint by as much as 200 times compared with the memory footprint of the legacy code. The resulting MPI/OpenMP algorithms can run up to six times faster than the MPI-based algorithm across benchmarks that use as many as 192,000 cores on Theta.

The team performed benchmarking of the memory and cluster modes of the KNL processor for the hybrid algorithms using graphene sheets with dimensions of 0.5 nm, 1.0 nm, 1.5 nm, 2.0 nm, and 5.0 nm. They benchmarked the memory and cluster modes of the KNL processor for the three algorithms using the 0.5-nm and 2.0-nm datasets.

Both hybrid algorithms exhibited better scalability (in terms of core counts) for both single and multi-node KNL systems. The team demonstrated the algorithms on as many as 3,000 Theta KNL nodes. These performance improvements extend the scope of chemical problems that can be treated with *ab initio* quantum chemistry methods in GAMESS. Furthermore, the insights gained by this work are applicable to a broader range of codes that solve nonlinear partial differential equations using matrix representations.

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

PI Volker Blum, Noa Marom
INST Duke University and Carnegie Mellon University
CODE FHI-aims, GAtor



The top 100 crystal structures of tricyano–1,4-dithiino[c]-isothiazole, as computed by GAtor and reranked by various DFT functionals and dispersion corrections. *Image: Álvaro Vázquez-Mayagoitia, Argonne National Laboratory; Farren Curtis, Noa Marom, and Timothy Rose, Carnegie Mellon University; Luca M. Ghiringhelli, Fritz Haber Institute of the Max Planck Society; Xiayue Li, Google; Saswata Bhattacharya, Indian Institute of Technology Delhi*

Organic and hybrid organic-inorganic materials have the potential to deliver advances in photovoltaic (PV) and other semiconductor applications. Accurate simulations of the structure and electronic properties of these materials would greatly accelerate efforts to identify the most promising organic-inorganic combinations. For this project, a research team from Duke University, University of North Carolina at Chapel Hill, Carnegie Mellon University, and Argonne National Laboratory worked to optimize two software packages—FHI-aims and GAtor—on Theta to enable efficient, large-scale predictions of the structure and properties of organic and organic-inorganic materials and interfaces.

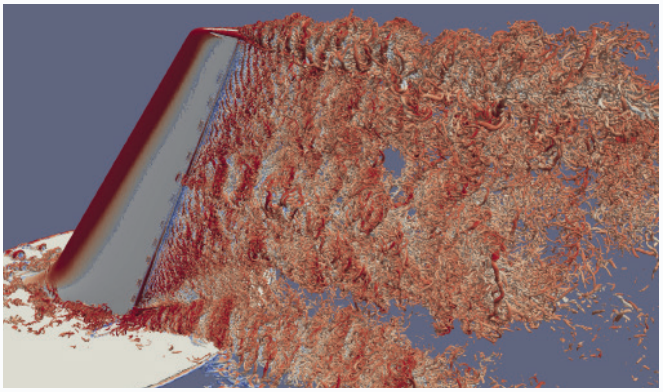
The FHI-aims code is a scalable all-electron electronic structure package capable of performing highly accurate quantum mechanical simulations—density functional theory (DFT) or beyond—of materials with model sizes up to and above 10,000 atoms. GAtor is a first-principles genetic algorithm (GA) designed to predict the structures of semi-rigid molecular crystals.

This project's methodological developments focused primarily on many-body perturbation theory, particularly on implementing the Bethe-Salpeter equation (BSE) for excitonic effects in FHI-aims. The team's initial scalability analysis of FHI-aims on Theta demonstrated surprisingly efficient scalability of the code's existing MPI parallelization on the Knights Landing architecture. Although the choice of compilers and compiler optimizations was not obvious, the team found that the gfortran compiler fared much better overall in tests for hybrid DFT. The researchers also performed a code analysis of FHI-aims to identify memory-intensive arrays, performing various memory optimizations to run the large calculations and implementing a lightweight memory tracking module. The team also optimized GAtor by using the mpi4py module instead of the subprocess module, allowing FHI-aims to be imported into Python as a library. Not only does this improvement enable GAtor to be truly massively parallel on Theta, but it also obviates any runs on mom nodes and reduces compute-node idle time.

The team's results demonstrated that Theta is well suited for the electronic structure-based simulation and prediction of new complex organic and organic-inorganic hybrid materials for PV and other applications. Theta proved capable of handling very large and complex structure models of organic-inorganic hybrid materials at the very demanding level of hybrid DFT. Theta and supercomputers like it may allow us to accurately predict the electronic properties of semiconductor materials with sufficient throughput and with the full predictive power of quantum mechanics.

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

PI Kenneth Jansen
INST University of Colorado Boulder
CODE PHASTA



Flow visualization through an isosurface of instantaneous Q criterion colored by speed. The analysis was executed on Theta using over 128Ki processes. *Image: Kenneth Jansen, University of Colorado Boulder*

Researchers from the University of Colorado Boulder, Rensselaer Polytechnic Institute, Argonne National Laboratory, and North Carolina State University explored the impact of applying the open-source, massively parallel computational fluid dynamics (CFD) analysis package, PHASTA, on Theta to advance computational modeling of turbulent flows around aerodynamic bodies, such as airplanes and wind turbines.

With previous allocations at the ALCF, the team performed highly resolved detached-eddy simulations of a vertical tail-rudder assembly with 12 synthetic jets. These simulations have shown excellent agreement on integrated quantities, like total force, as well as phase-averaged flow structures issued from the synthetic jets. This has yielded, for the first time, clear insight into the fundamental mechanisms of flow control.

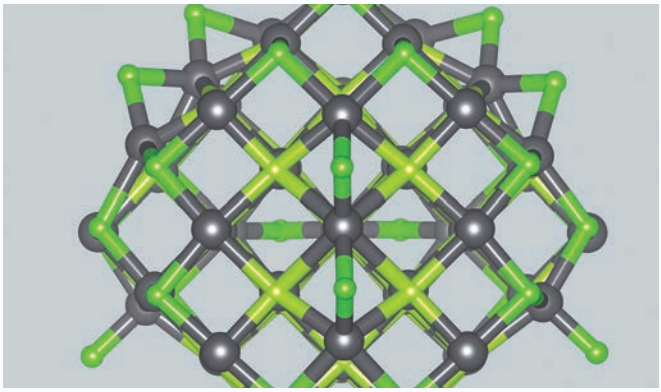
Using Theta, the team set out to extend these experiment-scale simulations to a Reynolds number eight times higher than previously explored, bringing the simulations substantially closer to flight scale. The simulations will help researchers better understand how the flow control structures and the jets that create them must be adjusted for Reynolds numbers. This capability sets the stage for the true flight-scale simulations that Aurora will make possible.

Achieving the highest possible portable performance on new architectures has been a major focus of PHASTA's development since its inception. Flexibility has been built into the code to make it highly adaptable to hardware and software advances. As part of the team's ESP work, the researchers used Intel's VTune performance profiling tool on Theta to confirm that a very high percentage of PHASTA's computationally intensive kernels were already highly vectorized. The team's runs on Theta showed a roughly 5x improvement in per-core performance compared to Mira.

In their studies on Theta, the researchers found that while adaptive, implicit unstructured grid CFD algorithms present formidable scaling challenges, they can be made both scalable and highly efficient in terms of science provided per CPU hour. By making complex features like adaptivity and implicit methods as efficient and scalable as possible, the team confirmed that realistic aircraft components, like a vertical tail/rudder assembly complete with active control, can be simulated accurately at wind tunnel scale and that these simulations are on the path to flight scale with Aurora.

First-Principles Simulations of Functional Materials for Energy Conversion

PI Giulia Galli
INST The University of Chicago and Argonne National Laboratory
CODE Qbox, WEST



PbSe nanoparticles were one of the systems investigated using the Qbox and WEST codes. *Image: Christopher Knight and Huihuo Zheng, Argonne National Laboratory; François Gygi, University of California, Davis; Giulia Galli and Marco Govoni, The University of Chicago and Argonne National Laboratory.*

A research team from Argonne National Laboratory, the University of Chicago, and the University of California, Davis, used Theta to investigate the electronic properties of several nanostructured materials for their potential use in solar and thermal energy conversion devices. In particular, the researchers focused on the opto-electronic properties of inorganic nanostructured samples for use in third generation solar cells. To do so, they used two open-source electronic structure codes: Qbox, an *ab initio* molecular dynamics code based on plane wave density functional theory (DFT); and WEST, a post-DFT code for excited-state calculations within many-body perturbation theory. The team's efforts to optimize the performance of these codes on Theta will play a key role in refining the road map for software development efforts targeting future large-scale computing resources such as Aurora.

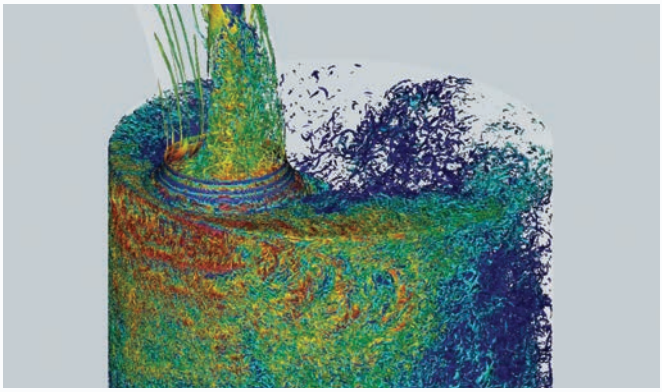
The ESP team's optimization work on Qbox largely focused on improving performance in the strong-scaling limit of the code by reducing or hiding the communication overheads associated with parallel dense linear algebra and 3D fast Fourier transformations (FFTs). Work included implementing data remap methods to efficiently redistribute data "on the fly" between ScaLAPACK process grids. These algorithms enable efficient calculation for separate phases of Qbox, where it is challenging to use a single context to solve different computational tasks. The performance improvements resulting from the team's optimizations significantly reduced the time to solution for hybrid-DFT calculations and allowed for efficient use of the full Theta system—enabling, for example, *ab initio* molecular dynamics simulations for systems with thousands of electrons.

For WEST, the researchers restructured the initial I/O phase to use a single-reader-broadcast algorithm, significantly improving weak scaling performance on the full Theta system. They also introduced additional levels of parallelism, exposing finer-grain work units that extended the strong scaling limits of the implemented algorithms. The team found that Theta node memory capacity allowed the smallest work unit (a single perturbation) to fit on one Knights Landing node (not possible on IBM Blue Gene/Q systems). These optimizations widen the scope of excited-state calculations, enabling more efficient use of large fractions of today's leadership computing resources, and potentially, of future exascale systems.

The project resulted in significant improvements in weak and strong-scaling performance for both codes on Theta. Many of the code optimizations implemented have also improved performance on relatively balanced architectures (e.g., Blue Gene/Q), where both codes already had good performance. This project's use of large fractions of available computing resources, combined with the reduced time to solutions, are enabling science-critical calculations that were not previously possible.

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

PI Christos Frouzakis
INST ETH Zurich
CODE Nek5000



DNS of the cold flow in the transparent combustion chamber (TCC) engine from the University of Michigan. The image shows vortical structures at 110 crank angle degrees after top dead center. *Image: Christos E. Frouzakis and George K. Giannakopoulos, ETH Zurich*

Modeling limitations can inhibit investigation of mixing and combustion in transient reacting jets. Researchers face a number of challenges in resolving the multitude of fast and spatially distributed variables. Direct numerical simulation (DNS) can solve these issues but the method depends on the availability of HPC architectures and efficient tools to harness their computational power. A team of researchers from ETH Zurich, Argonne National Laboratory, Aristotle University of Thessaloniki in Greece, and the University of Illinois at Urbana-Champaign used a reactive flow solver, built as a plugin to Nek5000, to simulate flow, mixing, and combustion phenomena in the gas phase, as well as on catalytic surfaces in laboratory-scale setups. Their ESP project focused on porting, tuning, and debugging the solver on Theta's Knight's Landing (KNL) architecture and implementing new algorithms to extend the modeling capabilities of the code for internal combustion engine applications.

The team's DNS code is based on the open-source solver, Nek5000, developed at Argonne and complemented by a plugin developed at ETH Zurich for the energy and chemical species governing combustion equations. Nek5000 is essentially a stand-alone code and compiles without problems on different systems. The reactive flow solver can account for detailed gas-phase chemistry and transport properties, as well as for detailed surface kinetics (catalytic combustion) in complex, variable geometries.

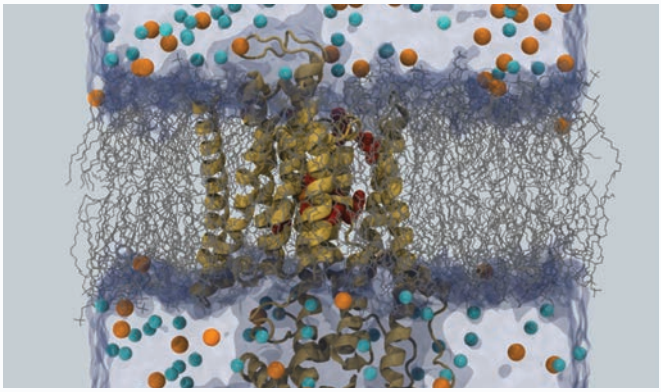
The researchers enhanced the code by (1) developing efficient mesh deformation algorithms and workflows suitable for complex geometries with moving piston and valves; (2) extending the characteristics method for efficient time integration with time-varying geometries to bypass standard Courant-Friedrichs-Lewy (CFL) constraints; (3) coupling the first two elements with the low-Mach-number reactive flow solver; and (4) performing "on the fly," high-order, scalable grid-to-grid interpolation to enable the use of multiple meshes during the simulation.

Their scaling studies on Theta revealed a 7.2x-per-node speedup in comparison with Blue Gene/Q. They found that Nek5000 scales well on Theta and can use all cores on a node using pure MPI. Aiming at simulations with more complex fuels—where the cost for chemical source terms and transport properties will increase with the number of species—the team developed a Matlab-based code that uses the standard Chemkin input files to generate optimized fuel-specific subroutines for the thermochemistry and transport properties kernels. The team achieved a speedup of 5.4x and 3.2x in the evaluation of the reaction rates and the transport properties, respectively. Overall, they achieved a 3.6x speedup of the total time to solution compared with the Chemkin subroutines.

Using the new capabilities, the research team performed science simulations of flow phenomena in an engine and of flow-flame and flame-wall interactions during fuel ignition in the main chamber by the hot reactive gases generated in a prechamber.

Free Energy Landscapes of Membrane Transport Proteins

PI Benoît Roux
INST The University of Chicago and Argonne National Laboratory
CODE NAMD



The Na/K pump (yellow) is a P-type ATPase that spans the plasma membrane of animal cells. It acts to maintain the ionic gradient (orange and blue spheres) that gives rise to the cell potential, a critical component of cell machinery and signal transduction. *Image: Brian Radak and Huan Rui, The University of Chicago*

Researchers from the University of Chicago, Argonne National Laboratory, and the University of Illinois at Urbana-Champaign developed and implemented a constant-pH molecular dynamics (MD) algorithm in the NAMD simulation engine, making it suitable for ambitious, cutting-edge biological applications—such as protein structure-function relationships—on next-generation supercomputers. For the first time, the researchers achieved constant-pH simulations of a membrane transport protein and used the results to analyze its free energy landscape for ion selectivity.

MD is widely used to investigate biochemical and biomolecular systems, thanks in part to advances in computational hardware over the last few decades. Conventional MD can investigate the behavior of a single protonation state, but it cannot address how to link the network of states together in a physically meaningful way. The vast majority of simulations today employ only rudimentary algorithmic approaches (so-called "brute force" MD), which only permit access to a small fraction of what the approach has to offer.

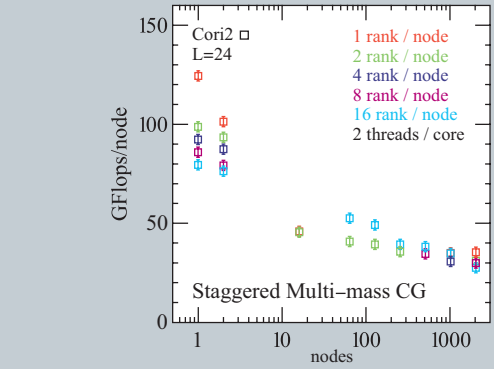
The NAMD code—written using the Charm++ parallel programming model—is used to simulate large systems (millions of atoms). NAMD is designed primarily for all-atom and coarse-grained MD with a focus on biomolecular applications. Like nearly all other codes of its kind, NAMD addresses the numerical integration problem by using a multiple-time step integrator with holonomic constraints on high-frequency degrees of freedom.

The team's constant-pH MD algorithm comprises three main parts: (1) specific Knights Landing optimizations for established NAMD functionality, (2) new features for constant-pH MD, and (3) a new analysis application, cphanalyze, that allows the constant-pH MD.

Optimizations were necessary at three levels: inter-node communications, thread-level parallelism, and single-instruction, multiple-data (SIMD) vectorization. The team's implementation included both modifications to low-level C/C++ applications for performance-sensitive activities, as well as high-level routines using the NAMD-Tcl interface. The new utility, cphanalyze, also implements state-of-the-art multistate reweighting techniques, leading to considerably better results compared with conventional methods. The code for this Python-based application is also made available with NAMD. The team plotted NAMD strong scaling on Theta and other machines versus nodes, sockets, and cores for 21-million- and 224-million-atom benchmarks. Compared to Mira, Theta is a factor of 10 faster per node. As a whole, these advances represent a new tool for the broader MD simulation community.

The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon

PI Paul Mackenzie
INST Fermilab
CODE Chroma, MILC, CPS



Weak scaling results for the team's double-precision, multi-mass HISQ (highly improved staggered quarks) conjugate gradient solver with the QPhiX library on KNL. The results are for a fixed problem size with varying MPI ranks per node and two threads per core. *Image: Carleton DeTar, University of Utah*

In physics, the muon—an elementary particle similar to an electron—acquires an "anomalous magnetic moment" (a source of the muon's magnetism) through fluctuations of particle fields. The experimental value of the muon's magnetic moment deviates from the Standard Model prediction by 3–4 standard deviations, potentially indicating new interactions not included in the Standard Model. The DOE is invested in refining the experimental measurement of the muon-anomalous magnetic moment (Fermilab's Muon g-2 experiment), but these efforts require an equal reduction in the theoretical error. With this ESP project, researchers from Fermilab, Columbia University, the University of Utah, and Thomas Jefferson National Accelerator Facility have developed lattice quantum chromodynamics (QCD) code, now running on Theta, to calculate the strong-interaction contribution to the Muon g-2.

The team's coding effort for QCD on Knights Landing (KNL) machines like Theta is structured around three primary code bases: Chroma, MILC, and the Columbia Physics System (CPS). Chroma is a C++ code used primarily in nuclear physics; it is based on a layered structure and supports both OpenMP threading on-node and internode communications via message-passing interface (MPI). The MILC code is written in C with MPI and OpenMP. The CPS code, written in C++, is based on the Grid framework which provides direct access to Theta's single-instruction, multiple-data (SIMD), multi-core, and multi-node parallelism. The MILC and CPS codes are used primarily in high energy physics.

For Chroma, the team's two main goals were to pursue (1) improvements to the QPhiX library to integrate it into a new Wilson-Clover Multi-Grid solver library aimed at KNL systems, and (2) investigation of performance portability using the Kokkos framework for parallel programming. The team contributed a chapter to the book *Exascale Scientific Applications: Scalability and Performance Portability*.

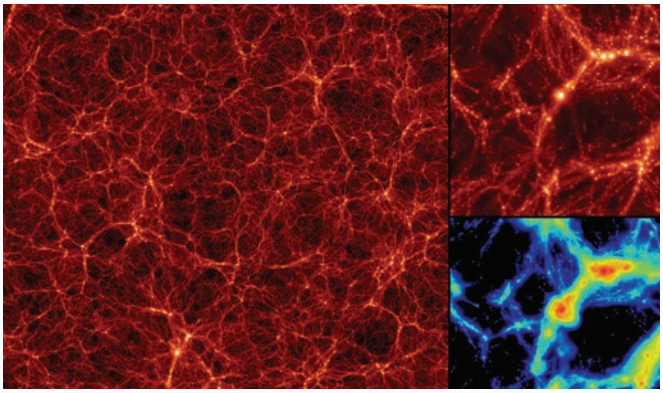
For MILC, the team added OpenMP threading directives to the most performance-critical parts of the code. They used the Intel VTune performance-analysis tool to assist in identifying portions of the code that would benefit from threading. They developed a KNL-specific conjugate gradient solver for their preferred quark formulation and added it to the QPhiX library.

For CPS, the researchers focused on achieving high multi-node KNL performance (typically 300 Gflops/sec) on Dragonfly (Theta) and Omnipath (Aurora) networks and on mitigating the unbalanced network that is provided with current KNL machines by using reduced precision communication and redistributing multi-right-hand-side solves to smaller sub-partitions (a 2.7x speedup).

This ongoing effort will ultimately require the ALCF's future Aurora system and a sustained software development effort to prepare for that next-generation machine.

Next-Generation Cosmology Simulations with HACC: Challenges from Baryons

PI Katrin Heitmann
INST Argonne National Laboratory
CODE HACC



This visualization shows baryon density (z = 0) from a 600 x 400 Mpc/h slice of depth 10 Mpc/h taken from a $(800\ \mathrm{Mpc/h})_3$ simulation with CRK-HACC. The subpanels show a zoomed-in 50 x 50 Mpc/h region, with the bottom subpanel showing the gas temperature. *Image: JD Emberson, Nicholas Frontiere, and the HACC team, Argonne National Laboratory*

The next generation of cosmological surveys covering the microwave, optical, and X-ray bands will start taking data soon. A major challenge in interpreting these new observations will be to disentangle astrophysical effects from fundamental physics. Efficient large-scale cosmology codes that incorporate baryons and feedback and that can scale up to the largest machines available will be crucial for the cosmology community. With this ESP project, a research team from Argonne National Laboratory, the University of Chicago, and the University of Renne built new capabilities for the extreme-scale Hardware/Hybrid Accelerated Cosmology Code (HACC) to allow simultaneous modeling of observations in all of these wavebands at high fidelity.

The team's work included developing and testing a new algorithm called Conservative Reproducing Kernel Smoothed Particle Hydrodynamics (CRK-SPH), which addresses some of the shortcomings of traditional SPH methods compared with adaptive mesh refinement (AMR) methods. The CRK-SPH scheme shows significant improvement in hydrodynamics problems involving shearing and mixing, in addition to shocks, while preserving the advantages of particle-based methods in performance and scalability. Before the start of this project, the HACC framework considered only gravitational forces; now it includes a hydrodynamics solver and a first set of sub-grid models, creating the CRKHACC framework.

The team extensively tested the CRK-SPH implementation on the KNL architecture. They verified the correctness of the implementation of the full-gravity-plus-CRK-SPH hydrodynamics capability by running the Santa Barbara cluster comparison benchmark for hydrodynamic cosmology codes. The results were found to be in very good agreement with AMR methods.

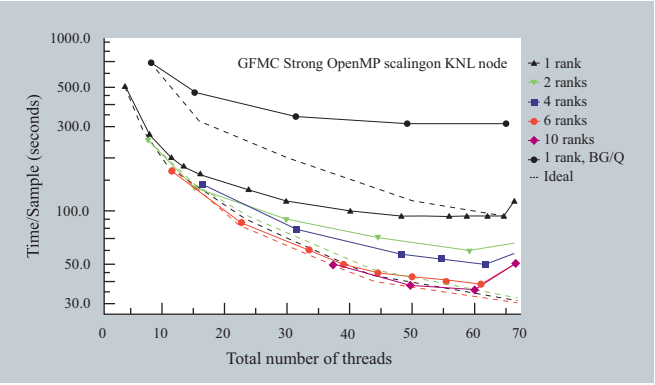
HACC (and therefore CRK-HACC) is designed to run on all available HPC architectures—95 percent of the code remains unchanged even when using radically different architectures. The team completed the optimization of the short-range solver (the 5 percent of the code that changes from platform to platform) for the KNL and demonstrated excellent performance and scaling results on the full machine.

The team achieved a major milestone with its "BorgCube" simulations. This involved performing two simulations, one with HACC and one using identical initial conditions with CRK-HACC, including baryonic physics. The simulations ran on 3,072 nodes of Theta (~90 percent of the initial machine) and evolved a total of ~25 billion particles in the case of the CRK-HACC run. The team can now carry out detailed studies of the impact of baryons on the matter distribution in the universe by comparing these two simulations.

Ultimately, the ESP team's work with both HACC and CRK-HACC demonstrated very good performance on Theta's KNL architecture. The CRK-HACC run on Theta will lead to important scientific insights, and it enabled the team to reach a significant milestone with regard to next-generation machines and the physics questions that can be studied. The continued development of a cosmological hydrodynamics code that can scale up to the largest machines available will have a major impact on upcoming cosmological surveys such as the Large Synoptic Survey Telescope, the Wide Field Infrared Survey Telescope, and the Dark Energy Spectroscopic Instrument.

Quantum Monte Carlo Calculations in Nuclear Theory

PI Steven Pieper
INST Argonne National Laboratory
CODE GFMC



Scaling of GFMC calculations on KNL nodes and Theta. *Image: Alessandro Lovato, Ewing Lusk, Maria Piarulli, Steven Pieper, and Robert Wiringa, Argonne National Laboratory*

Solving the many-body Schrödinger equation is a challenging problem in nuclear physics because of the non-perturbative nature and the strong spin-isospin dependence of the nuclear forces. For many scientists, Quantum Monte Carlo (QMC)—in particular, Green's function Monte Carlo (GFMC)—is the many-body method of choice for solving the problem. GFMC allows users to solve the nuclear Schrödinger equation with the required one percent accuracy for both the ground- and the low-lying excited states of $A \leq 12$ (A is the number of nucleons) nuclei. For this ESP project, a team of researchers from Argonne National Laboratory used Theta to make GFMC calculations, finding good agreement with data and strong scaling for the application.

The GFMC application has been used for many years, undergoing steady improvements to take advantage of each new generation of parallel machines. GFMC provides *ab initio* calculations of the properties of light nuclei by solving the many-body Schrödinger equation using realistic two- and three-nucleon interactions. It is generally recognized as the most reliable method for modeling nuclei containing six to 12 nucleons.

GFMC displayed strong MPI scaling to the full Theta machine and good OpenMP scaling to the number of threads (cores) available to a given MPI rank. The team identified several OpenMP errors and inefficiencies using the Intel compiler with the Cray operating system. They also found that the AVX512 instructions did not substantially increase the speed of GFMC's most time-intensive operations because the team was working with COMPLEX arrays, which, by the Fortran standard, have pairs of real and imaginary numbers. Thus, they did not meet the AVX requirement of having unit stride.

The program was already making good use of OpenMP, but the team made some additional improvements and added subroutines to compute the new χEFT potentials. Because their use of the C preprocessor for Fortran source was not supported by the Cray compiler, they needed to have the Makefile invoke a script that ran the Fortran through the C compiler and captured the modified Fortran source, which was then given to the Cray Fortran compiler. The team had no significant problems running GFMC on Theta using the Intel compiler, with the exception of changes to the Makefiles to use the Cray compiler. Ultimately, the project proved valuable in allowing the research team to learn how to use Theta and to complete calculations for new science work that resulted in a paper published in *Physical Review Letters*.

Preparing for the Future of HPC

Argonne's Joint Laboratory for System Evaluation (JLSE) enables researchers to access and explore next-generation hardware and software platforms.

Established by the ALCF and the Mathematics and Computer Science (MCS) Division, the JLSE centralizes Argonne's research activities aimed at evaluating future extreme-scale computing systems, technologies, and capabilities.

JLSE users leverage existing infrastructure and 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.

By providing access to leading-edge computing resources and fostering collaborative research, the JLSE enables researchers to address Argonne and DOE needs in a variety of areas, which include:

- Improving science productivity on future hardware and software platforms
- Providing an avenue for Argonne researchers to work collaboratively with HPC vendors on prototype technologies for petascale and beyond
- Investigating alternative approaches to current and future system deployments
- Maintaining a range of hardware and software environments for testing research ideas
- Helping to drive standards on benchmarks, programming models, programming languages, memory technologies, etc.

JLSE Systems

The joint laboratory provides users with access to several diverse testbeds, including:

Intel Xeon Phi (Knights Landing) and Xeon (Skylake) Clusters

IBM Power System S822LC

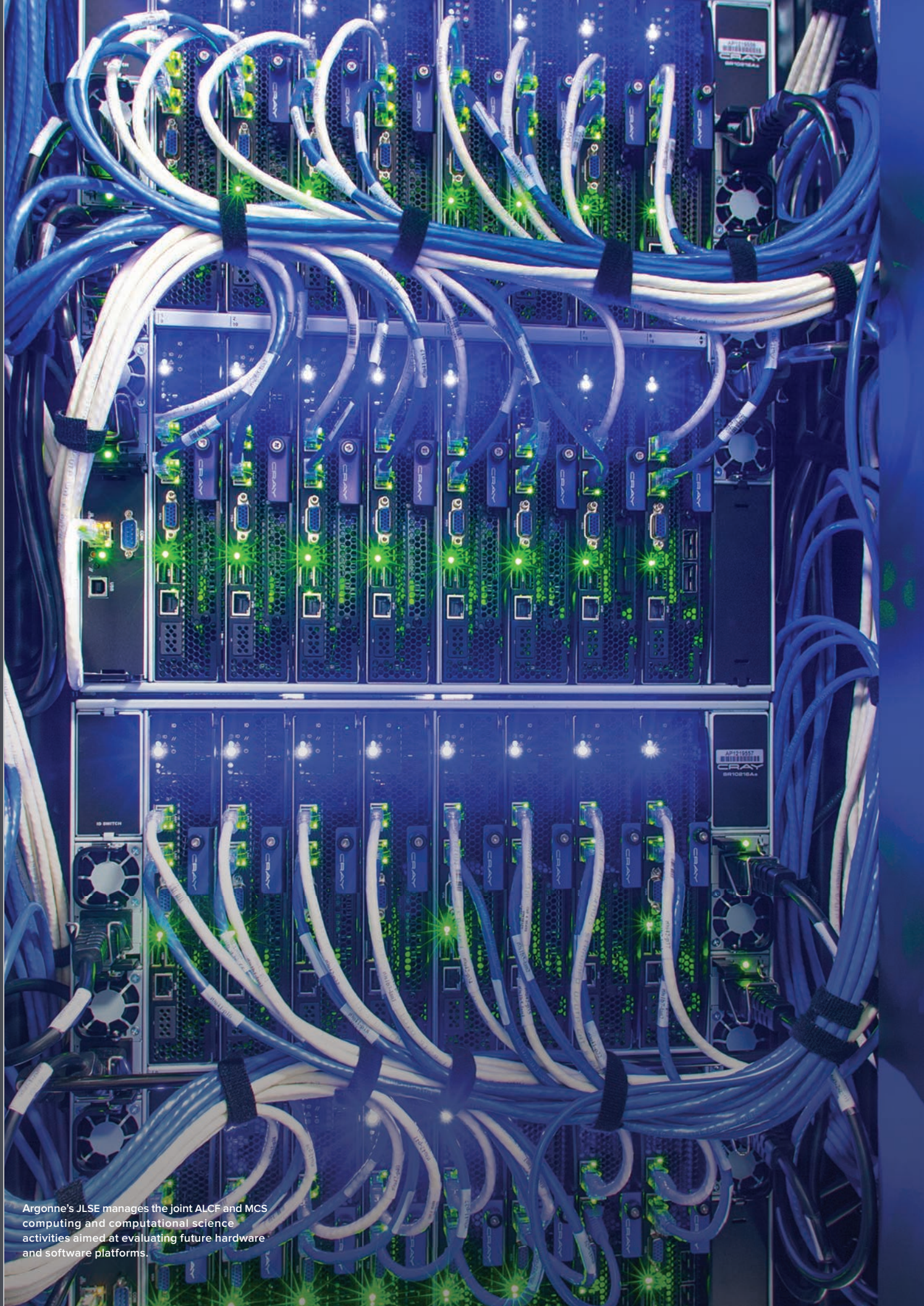
NVIDIA DGX–1 System (Volta GPUs)

AppliedMicro X-C1 Server ARM Development Platform

Atos Quantum Learning Machine

IBM Elastic Storage Server GL6

Lustre Testbed



Argonne's JLSE manages the joint ALCF and MCS computing and computational science activities aimed at evaluating future hardware and software platforms.

JLSE Projects

In 2017, the JLSE supported more than 374 users participating in 44 projects. The following summaries represent a sampling of current JLSE projects.

ALCF Data Science Program

PI Venkatram Vishwanath, Argonne National Laboratory

Research teams from ALCF Data Science Program use JLSE resources to explore and improve data science techniques, such as data mining, graph analytics, machine learning, and complex and interactive workflows.

CANDLE Application Development

PI Rick Stevens, Argonne National Laboratory

Using the NVIDIA DGX–1 system and other JLSE computing resources, researchers are developing the CANcer Distributed Learning Environment (CANDLE), a computational framework designed to facilitate breakthroughs in the fight against cancer.

Improving MPICH Performance

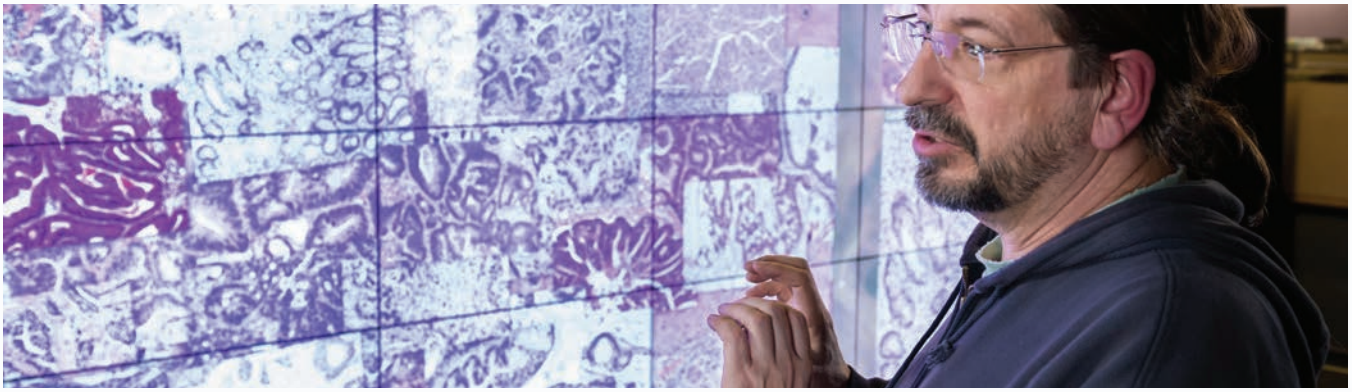
PI Pavan Balaji, Argonne National Laboratory

A number of MPI Chameleon (MPICH) improvements were tested on JLSE systems, including the memory scalability of MPI communicators by exploiting regular patterns in rack-address mapping; enhanced threading support through locking optimizations; and communication-aware thread scheduling.

Artificial Neural Network for Spectral Analysis

PI Kirill Prozument, Argonne National Laboratory

A research team is using the JLSE's Atos Quantum Learning Machine and other resources to develop an artificial neural network for spectral analysis called Spectranne. This tool will automate the analysis of vast amounts of data being produced by state-of-the art chirped-pulse spectroscopy experiments.



Led by Rick Stevens, Argonne's Associate Laboratory Director for Computing, Environment and Life Sciences, the CANDLE project is using advanced computing systems, including JLSE resources, to develop a deep neural network code for cancer research.

ALCF Early Science Program

PI Tim Williams, Argonne National Laboratory

Research teams from the ALCF Early Science Program (ESP) use JLSE resources to prepare and optimize applications for the next-generation supercomputers in advance of the systems being available. For example, researchers from the Theta ESP used JLSE's Intel Xeon Phi cluster to work on single-node optimization, focusing on memory modes and vectorization.

LLVM and CLANG Improvements

PI Hal Finkel, Argonne National Laboratory

Researchers used the JLSE's IBM Power systems to advance low-level virtual machine (LLVM) compiler development. The instruction set architecture for these systems is the same as for the IBM Blue Gene/Q system, different only in their vectorization. LLVM and CLANG builds were carried out on Intel Xeon Phi systems for quality assurance purposes. Researchers can complete these builds in 10 minutes using JLSE resources (compared to hours on a laptop).

Big Data and Programming Models

PI Tom Peterka, Argonne National Laboratory

Researchers are using JLSE testbeds to study the layering of HPC programming models beneath big data programming models. Specifically, they are researching the development of a software enviroment with a Spark user interface (Java and Scala) that can run on a supercomputer, cluster, or cloud with a backend for executing data-intensive communication patterns.

Deep Learning Frameworks Performance

PI Yasaman Ghadar, Argonne National Laboratory

Researchers are using JLSE systems to understand the performance of different machine learning frameworks that have implemented deep learning and neural networks on Knights Landing systems. As part of this work, they are using different parameters, such as batch size and epochs, to evaluate time to solution and accuracy of the frameworks.

Argo: An Exascale Operating System

PI Swann Perarnau, Argonne National Laboratory

Argo is a new exascale operating system and runtime system designed to support extreme-scale scientific computation. Researchers from the Argo project used JLSE resources to prototype the GlobalOS distributed resource management platform and to evaluate the performance of NodeOS. They also used the laboratory's testbeds to develop and optimize a lightweight, low-level threading and task framework for OpenMP and other programming models (Cilk, Quark, Charm++).

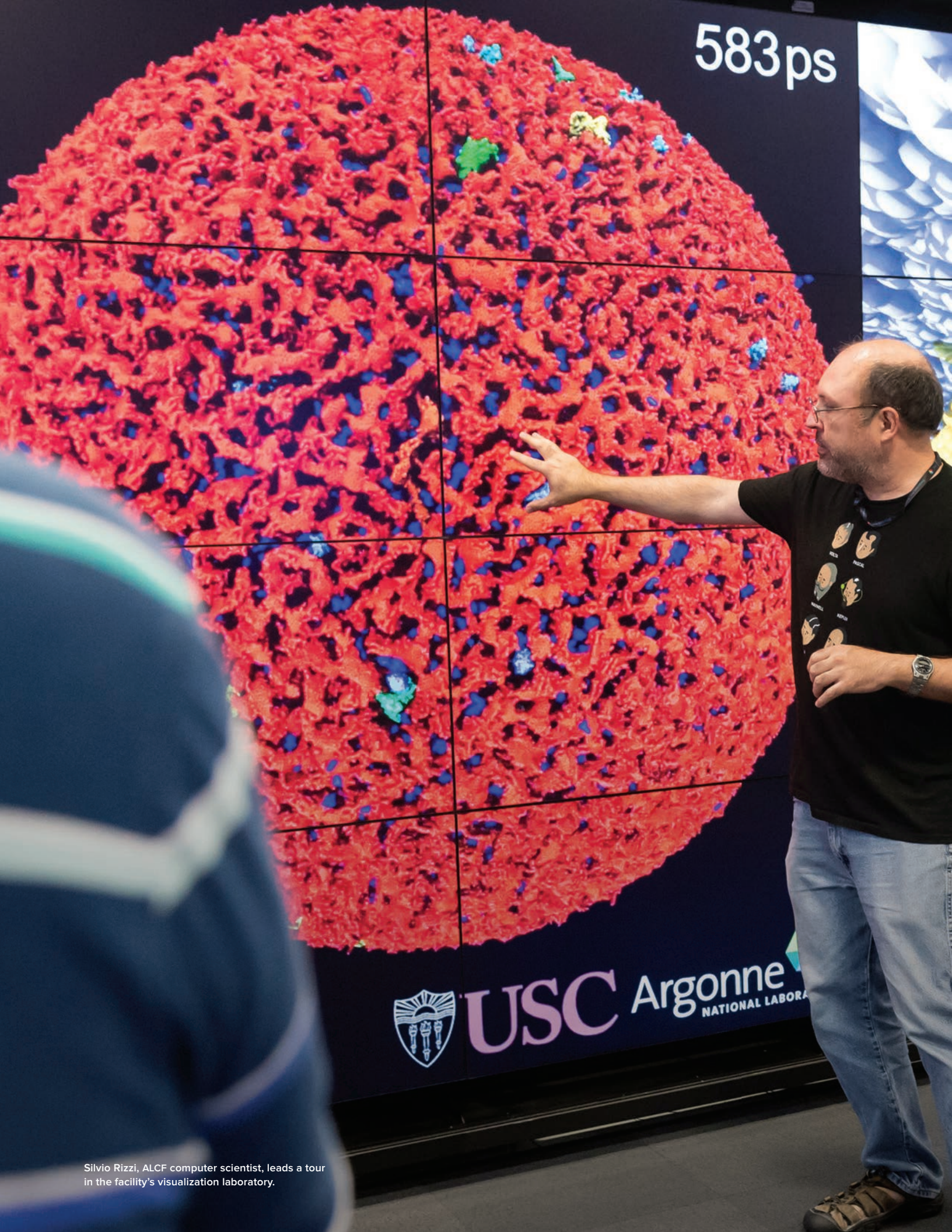
Enhancing the TAU Toolkit

PI Sameer Shende, University of Oregon and Paratools, Inc.

Researchers ported the Tuning and Analysis Utilities (TAU) performance analysis toolkit to various instruction set architectures and other JLSE systems, including AppliedMicro's X-Gene ARM64, Intel Xeon Phi clusters, and IBM Power systems. The team validated support for OpenMP profiling via the OpenMP tools interface and vectorization intensity on JLSE systems.

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 community of researchers who can use them for scientific computing.



Silvio Rizzi, ALCF computer scientist, leads a tour in the facility's visualization laboratory.

Partnering with Industry for High-Impact Research

ALCF computing resources and expertise are powerful tools for driving innovation and competiveness in the private sector.

Leadership computing systems like Mira and Theta allow industry users to tackle computational problems that are impossible to address on their internal computing systems.

Equipped with advanced capabilities for simulation, data, and learning, ALCF supercomputers help companies expedite R&D efforts for many applications, including combustion engines, novel materials for energy and medicine, and fusion energy devices, to name a few.

With access to ALCF systems and expertise, industry researchers can create higher fidelity models, achieve more accurate predictions, and quickly analyze massive amounts of data. The results enable companies to accelerate critical breakthroughs, verify uncertainties, and drastically reduce or eliminate the need to build multiple prototypes.

Ultimately, industry partnerships with the ALCF help to strengthen the nation's innovation infrastructure and expand the use of HPC resources to improve competitiveness.

To broaden this impact, the ALCF Industry Partnerships Program, led by David Martin, is focused 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 leadership computing resources and leverage ALCF expertise.

The ALCF works closely with other Argonne user facilities and divisions, including the Technology Development and Commercialization Division, to facilitate opportunities for collaboration across the laboratory. This collaborative approach allows the ALCF to present a more complete picture of Argonne's resources, resulting in broader engagements across the laboratory with a number of companies.

Additionally, Martin 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 a few companies are using ALCF resources to advance their R&D efforts.

Simulation

Kinetic Simulation of Field-Reversed Configuration Stability and Transport

PI Sean Dettrick, TAE Technologies

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.

Data

DIII-D Computing

PI David Schissel, General Atomics

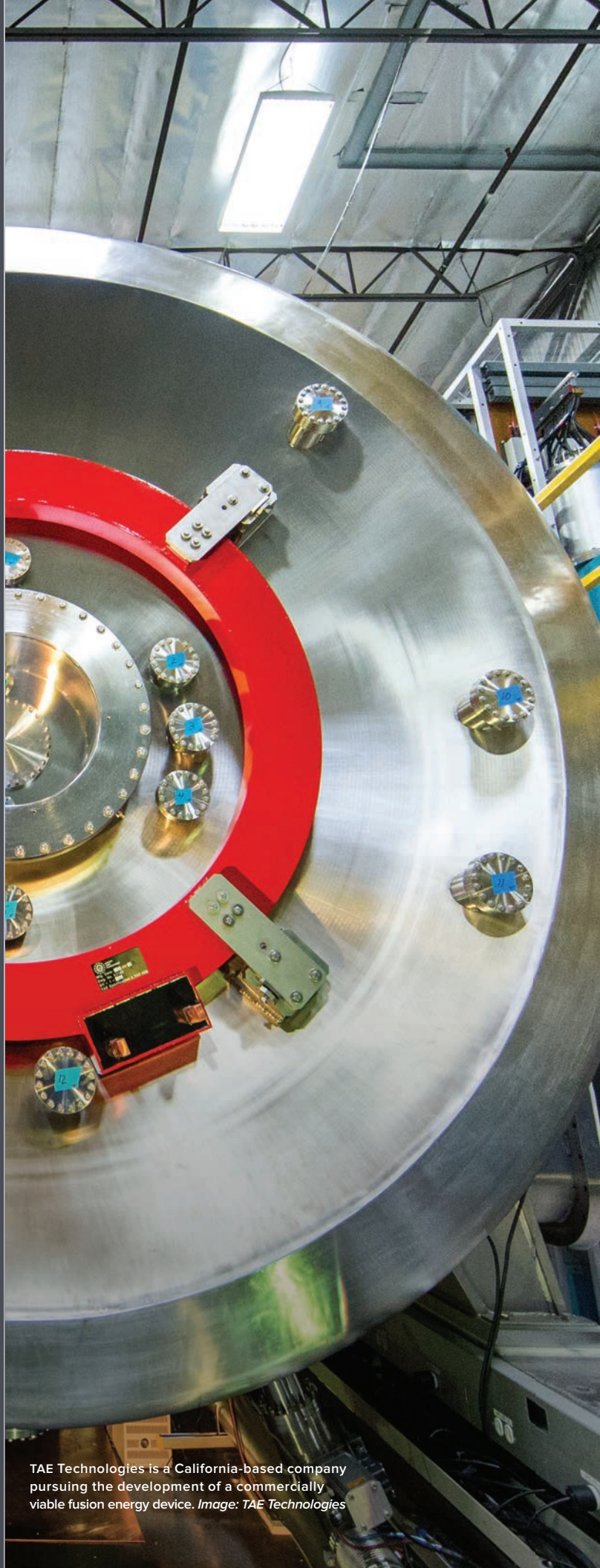
Researchers from the DIII-D National Fusion Facility, at General Atomics, are using ALCF computing resources to perform near-real-time data analysis to advance their experimental efforts to optimize the tokamak approach to fusion energy production. By automating and shifting a data analysis step to the ALCF, the team has created a virtual iterative loop that helps scientists to rapidly calibrate their fast-paced plasma physics experiments.

Learning

Enabling Multiscale Physics for Industrial Design Using Deep Learning Networks

PI Rathakrishnan Bhaskaran, GE Global Research

A team from GE Global Research is 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.



TAE Technologies is a California-based company pursuing the development of a commercially viable fusion energy device. *Image: TAE Technologies*

Shaping the Future of Supercomputing

ALCF researchers lead and participate in several strategic activities that aim to push the boundaries of what's possible in computational science and engineering.

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 are involved in the testing and development of new HPC hardware and software, and work closely with the researchers who use these leading-edge systems to pursue scientific breakthroughs. This experience gives the ALCF a unique perspective on the methods, trends, and technologies at the bleeding edge of HPC.

Leveraging this knowledge and expertise, ALCF researchers contribute to many HPC community efforts to advance the use of supercomputers for discovery and innovation.

For example, the ALCF is a key player in DOE's Exascale Computing Project, a multi-lab initiative to plan and prepare for a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.

In addition, ALCF staff members are helping to develop the software, standards, and benchmarks needed to drive continued improvements in supercomputing performance. They also frequently deliver talks and participate in numerous topical workshops and meetings, using the opportunities to promote the ALCF as a world-class user facility.

Prasanna Balaprakash, ALCF computer scientist, delivers a talk at Argonne's Machine Learning Workshop for students and postdocs.

Community Activities

SC17

As home to the ALCF and the Mathematics and Computer Science (MCS) Division, Argonne again had a strong presence at the HPC community's premier annual conference—SC17, the International Conference for High-Performance Computing, Networking, Storage and Analysis. This year's event took place in November in Denver, Colorado. More than 40 Argonne researchers attended SC17 to share their HPC work and knowledge through a wide range of activities, including technical paper presentations, invited talks, workshops, panel discussions, and tutorials. In addition, the ALCF organized an annual industry lunch at SC17, providing an opportunity for ALCF leadership to meet with industry users of HPC to explore potential partnerships and discuss issues like workforce development.

SIGHPC Chapter Leadership

ALCF staff members are advancing the HPC community through their involvement in the Association for Computing Machinery's Special Interest Group on High-Performance Computing (ACM SIGHPC). Richard Coffey of the ALCF serves as the chair of the SIGHPC Education Chapter (SIGHPCEDU). In 2017, SIGHPCEDU merged with the International HPC Training Consortium to build a combined collaborative community focused on the development, dissemination, and assessment of HPC training and education materials. The ALCF's William Scullin chairs SIGHPC's Systems Professionals Chapter, a group that supports the interests and needs of systems administrators, developers, engineers, and other professionals involved or interested in the operation and support of HPC systems.

Petascale Science Sessions

ALCF staff members co-organized special petascale computing sessions at two major scientific conferences this year. At the 2017 March Meeting of the American Physical Society, in New Orleans, Louisiana, Nichols Romero of the ALCF collaborated with colleagues from OLCF, NERSC, and the National Institute of Standards and Technology to organize a session titled "Petascale Science and Beyond: Applications and Opportunities for Materials Science." In August, the ALCF's Yuri Alexeev worked with staff from other national laboratories, the U.S. Department of Defense and the U.S. Army Corps of Engineers, to help organize the petascale science session, "Extending Accuracy and Scales with Emerging Computing Architectures and Algorithms," at the American Chemical Society National Meeting and Exposition in Washington, D.C.

HPC Standards, Benchmarks, and Technologies

ALCF researchers are actively involved in developing standards, benchmarks, and technologies that help drive continued improvements in supercomputing performance. Staff activities include contributing to the C++ Standards Committee (Hal Finkel); the OpenMP Architecture Review Board (Kalyan Kumaran); the OpenMP Language Committee (Ray Loy); the OpenFabrics Interfaces Working Group (Paul Coffman); the HPCXXL User Group (Loy); and the Standard Performance Evaluation Corporation (Kumaran). ALCF staff members also serve on the boards of Open Scalable File Systems, Inc. (Kevin Harms), a nonprofit dedicated to supporting the Lustre file system; and the LLVM Foundation (Finkel), a nonprofit focused on supporting the LLVM project and advancing the field of compilers and tools.

Argonne's Machine Learning Workshop provided an introduction to machine learning and an opportunity to discuss cross-disciplinary collaborations.

Intel Xeon Phi User Group

As one of the founding members of the Intel Xeon Phi User Group (IXPUG), the ALCF is active in the group's mission 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, such as Theta. David Martin of the ALCF currently serves as president of the IXPUG Steering Committee. In 2017, IXPUG held eight significant events, including the group's annual meeting. In addition, IXPUG held workshops and birds-of-a-feather sessions at the International Supercomputing Conference (ISC) and at SC17. Regional and topic-specific meetings rounded out the year's activities.

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.

Exascale Crosscut Review

In 2017, ALCF, NERSC, OLCF, and ESnet completed the Exascale Requirements Reviews: Crosscut Report. This report highlighted key findings across the DOE Office of Science drawn from the six Exascale Requirements Review Reports published in 2016 and 2017. These findings addressed needs in computing, data, software and application development, and training and workforce development. The Crosscut Report, the six Exascale Requirements Review Reports, and references (including DOIs) can be found on the exascaleage.org website.

Machine Learning Workshops

In 2017, ALCF staff members contributed to two Argonne workshops focused on machine learning. In March, a two-day workshop focused on the wide-ranging use of machine learning across the lab, highlighting opportunities for cross-disciplinary discussion and collaboration. The workshop also offered an introductory hands-on tutorial session for researchers of all backgrounds on using machine learning for their research. In July, a similar machine learning workshop was held for students at the laboratory.

Performance Portability

Tim Williams of the ALCF partnered with colleagues from NERSC and OLCF to create and deploy a performance portability website (performanceportability.org). The website provides resources and best practices for achieving performance portability across the DOE Office of Science computing facilities. The collaborative effort included leading a breakout session at the 2017 DOE Centers of Excellence Performance Portability Meeting, in Denver, Colorado, to demonstrate and get feedback on the new website.

Engaging Current and Future HPC Researchers

The ALCF provides training opportunities to prepare researchers to efficiently use its leadership computing systems, while also participating in outreach activities that aim to cultivate the HPC community of tomorrow.

From informing ALCF users of new approaches and tools for leadership supercomputers to introducing students to exciting career possibilities in computing-related fields, education and outreach are critical parts of the ALCF's mission.

For the facility's user community, outreach is focused on offering expert-guided training opportunities to educate users about the tools, computational resources, and services available to them in support of scientific discovery.

In 2017, the ALCF organized and hosted several events to prepare researchers to use Theta, the facility's new Intel-Cray system. This included a hands-on workshop that allowed attendees to test and optimize applications on Theta; interactive videoconferences that connected users with experts from Intel and Cray; and a tutorial series focused on many-core tools and techniques.

ALCF staff members also volunteer for a wide variety of outreach activities directed at students. Through participation in events like Hour of Code and Argonne's Introduce a Girl to Engineering Day, ALCF researchers get an opportunity to spark students' interest in coding, computer science, and the power of supercomputing.

In addition, the facility hosts an annual summer student program that gives college students a unique opportunity to work with some of the world's most powerful computing resources. The students collaborate with ALCF staff members on real-world research projects in such areas as system administration, data analytics, and computational science.

Emily Shemon, ALCF computational scientist, speaks with middle school students at the CodeGirls at Argonne camp.

Inspiring Students

CodeGirls@Argonne Camp

In August, Argonne hosted nearly two dozen seventh- and eighth-grade girls for a two-day camp aimed at teaching the fundamentals of coding in the Python programming language. The girls also met with computer scientists at the lab and toured the ALCF.

Hour of Code

As part of Code.org's annual Hour of Code event in December, several ALCF staff members visited Chicago-area schools to spark interest in computer science and coding. Working with grades ranging from kindergarten to high school, the ALCF volunteers led a variety of activities designed to teach students the basics of coding. The global outreach campaign aims to expand participation and increase diversity in computer science.

SC17 Student Cluster Competition

The ALCF co-sponsored the Chicago Fusion team in the Student Cluster Competition at SC17, 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, Maine South High School, and Adlai Stevenson High School. With financial and technical support provided by Argonne, Intel, Calyos, NVIDIA, and the National Science Foundation, the team fared well at this year's event, earning first place in an exercise that involved using a mystery application. To prepare for the competition, ALCF researchers worked closely with the students to provide logistical, setup, and application support.

Summer Coding Camp

In July, ALCF staff taught and mentored 30 area high school students at Argonne's Summer Coding Camp. The camp curriculum promotes problem-solving and teamwork skills through hands-on activities, such as coding with Python and programming a robot via a Raspberry Pi. The camp is a joint initiative of the ALCF and Argonne's Educational Programs Office.

Joe Insley, ALCF visualization team lead, works with high school students at Argonne's Summer Coding Camp.

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 39 students ranging from college freshmen to PhD candidates through programs like DOE's Science Undergraduate Laboratory Internship and Argonne's Research Aide Appointments. From exploring big data analysis tools to developing new HPC capabilities, many of this year's interns had the opportunity to gain hands-on experience with some of the most powerful supercomputers 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

Through participation in Argonne events like Introduce a Girl to Engineering Day and the Science Careers in Search of Women conference, ALCF staff members have the opportunity to connect with young women and introduce them to potential career paths in science, technology, engineering, and mathematics (STEM). The ALCF also promotes STEM careers to women through contributions to Argonne's Women in Science and Technology group, the Anita Borg Institute, the Grace Hopper Celebration of Women in Computing, and the Rocky Mountain Celebration of Women in Computing.

Training Users

ALCF Computational Performance Workshop

Held in May, the ALCF Computational Performance Workshop was designed to help users prepare and improve their codes for ALCF supercomputers, including Theta, the facility's new Intel-Cray system. The intensive, hands-on workshop connected both current and prospective users with the experts who know the systems inside out—ALCF computational scientists, performance engineers, data scientists, and visualization experts, as well as invited guests from Intel, Cray, Allinea (now part of ARM), ParaTools (TAU), and Rice University (HPCToolkit). With dedicated access to ALCF computing resources, the workshop provides an opportunity for attendees to work directly with these experts to test, debug, and optimize their applications on leadership-class supercomputers. One of the ALCF workshop's goals is to help researchers demonstrate code scalability for INCITE and ALCC project proposals, which are required to convey both scientific merit and computational readiness.

ALCF Getting Started Videoconferences

The ALCF hosts several virtual "Getting Started" sessions throughout the year to help new and existing users get their projects up and running on ALCF computing resources. Led by ALCF staff, these interactive videoconferences cover system architectures, code building, job submissions, data storage, compilers, and other topics.

ATPESC 2017

In July and August, the ALCF ran its fifth Argonne Training Program on Extreme-Scale Computing (ATPESC), a two-week training program for 65–70 early career researchers and aspiring computational scientists. ATPESC's seven program tracks focus on HPC methodologies that are applicable to current and future machine architecture, including exascale systems. Renowned scientists and HPC experts provide the technical lectures, hands-on exercises, and dinner talks. To further extend ATPESC's reach, ALCF staff produces and uploads video playlists of ATPESC content to Argonne's YouTube training channel. More than 60 hours from the 2017 course were uploaded in September. Since 2013, ATPESC's inaugural year, these videos have been viewed more than 21,000 times.

ALCF researcher Ying Li (left) works with an attendee at the ALCF Computational Performance Workshop, an annual training event dedicated to helping users improve application performance on the facility's supercomputers.

Best Practices for HPC Software Developers

In 2017, the ALCF, OLCF, NERSC, and the Interoperable Design of Extreme-Scale Application Software (IDEAS) project continued to deliver its 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 Python in HPC, Managing Defects in HPC Software Development, and the Better Scientific Software (BSSw) community website.

Many-Core Training Offerings

To help support and expand the Theta user base, the ALCF introduced a tutorial series and a live-presentation webinar series aimed at efficient use of the many-core system. The "Many-Core Tools and Techniques" tutorial series covered topics such as architectural features, tuning techniques, analysis tools, and software libraries. The "Many-Core Developer Sessions" webinar series was created to foster discussion between actual developers of emerging hardware and software, and the early users of that technology. Speakers in this series have included developers from Intel and Allinea (ARM), covering topics such as AVX–512, Vtune, TensorFlow, and debugging.

Preparing for KNL

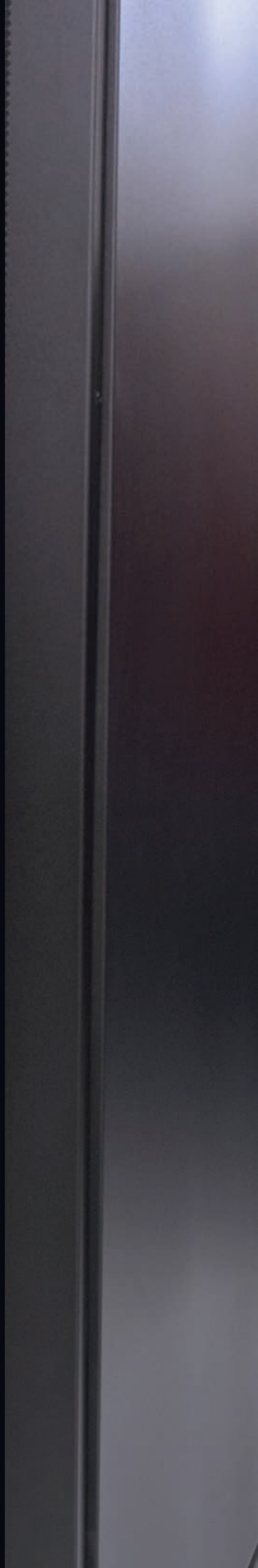
The ALCF organized a three-part videoconference series that convened Intel and Cray experts and early Theta users (project team members from the Theta ESP and the ALCF Data Science Program) to discuss and address specific Knights Landing (KNL)-related issues encountered on Theta. In addition, Intel and the ALCF curated a collection of publicly available videos aimed at getting users up and running on KNL hardware.

Scaling to Petascale Institute

In June, the ALCF, the National Center for Supercomputing Applications/Blue Waters Project, NERSC, OLCF, Stony Brook University, and the Texas Advanced Computing Center organized a weeklong "Scaling to Petascale" Institute. The goal was to prepare participants to scale simulations and data analytics programs to petascale-class computing systems in support of computational and data-enabled discovery for all fields of study. Organizers worked to facilitate the participation of a large national audience by streaming the sessions to a number of host sites, including the ALCF. Sessions were also webcasted on YouTube Live (recordings of the presentations were made available after the event). In total, more than 400 people attended via the host sites, and more than 200 people registered to watch the sessions via YouTube Live.

EXPERTISE AND RESOURCES

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



The ALCF's computing resources are located in Argonne's Theory and Computing Sciences Building.

The ALCF Team

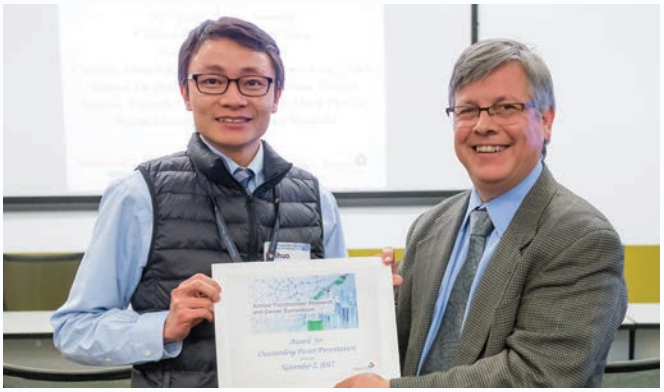
The ALCF's talented and diverse staff make the facility one of the world's premier centers for computational science and engineering.

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
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 scientifically productive.

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



Huihuo Zheng (left) of the ALCF received an award for Outstanding Poster Presentation at Argonne's annual postdoc symposium. The award was presented by John Quintana (right), Argonne's Deputy Director for Operations and Chief Operations Officer.

Zheng Recognized at Postdoctoral Symposium
Huihuo Zheng, ALCF postdoctoral appointee, received an award for Outstanding Poster Presentation at Argonne's Postdoctoral Research and Career Symposium, an annual event that showcases the scientific research of postdocs and graduate students from Argonne, Fermilab, and Chicago-area universities.

Zheng's poster, "Performance Optimization of WEST and Qbox on Intel Knights Landing," communicated findings from a project in the ALCF's Theta Early Science Program.

Ramprakash Receives Mentoring Award
In recognition of her mentoring and outreach efforts, ALCF Deputy Division Director Jini Ramprakash received the 2017 Motivator Award from the Association of Women in Science (AWIS) Chicago Chapter.

At Argonne, Ramprakash regularly participates in and helps organize laboratory initiatives designed to inspire young women to enter STEM fields. This includes serving as a volunteer and mentor for Argonne's annual Introduce a Girl to Engineering Day and the Science Careers in Search of Women conference, which are supported by the lab's Women in Science and Technology (WIST) program. Both of these events invite young female students to Argonne for hands-on activities, tours, and interaction with women mentors from the laboratory.

Ramprakash is also an active contributor to Systers, an online community of women in technical computing roles. As a volunteer for Systers-supported initiatives, like the Google Summer of Code and Code-In programs, she mentors and consults young women working on real open-source software development projects.

In addition, Ramprakash serves on review committees for the Grace Hopper Celebration of Women in Computing, the world's largest gathering of women technologists. Here, she represents Argonne, working to grow the participation of other national laboratories, and connecting women in STEM with potential career opportunities.

Williams Contributes to Book on Exascale Applications
Tim Williams, ALCF Deputy Director of Science, collaborated with colleagues from OLCF and NERSC to co-edit a new book titled, *Exascale Scientific Applications: Scalability and Performance Portability*.

Published in November 2017, the book provides practical programming approaches for scientific applications on exascale computer systems, as well as strategies for making applications performance portable. It includes contributions from leading experts involved in the development and porting of scientific codes for current and future high-performance computing resources.

Staff Members Honored with Pacesetter Awards
In 2017, five ALCF staff members received Argonne Pacesetter Awards, which are given to employees who have shown extraordinary initiative and dedication in their work at the laboratory.

Beth Cerny was recognized for her role in delivering reports, a website, and supporting materials for the DOE Office of Science Exascale Requirements Reviews.

Kevin Harms was recognized for his collaborative efforts with Argonne's Virtual Engine Research Institute and Fuel Initiative (VERIFI) to scale the CONVERGE application on ALCF systems.

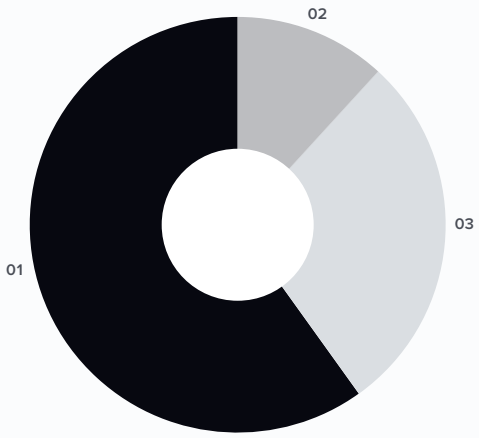
Christopher Knight, Vitali Morozov, and Scott Parker were recognized for their work on testing early versions of the Intel Xeon Phi (Knights Landing) chip.

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 2017.

ALCF STAFF NUMBERS



01 Staff Members

83

02 Postdoctoral Researchers

16

03 Summer Students

39

Ben Allen
HPC Systems Administrator

Between the ALCF and Argonne's Joint Laboratory for System Evaluation (JLSE), Ben has been instrumental to the operation of some of the most advanced HPC systems in the world. As the experimental systems lead for JLSE, he supports several leading-edge testbeds that enable Argonne researchers and ALCF Early Science Program teams to carry out studies that will ultimately help to improve science productivity on future hardware and software platforms.

In 2017, Ben played a critical role in the ALCF's deployment of Theta, assisting with the integration of the new system from the point of acceptance until it entered production mode in July. In preparation for Aurora, he has worked closely with vendors, Intel and Cray, to provide guidance on an ideal software stack for the ALCF's next-generation system. Ben's work with Aurora has led him to investigate the development of combined provisioning and configuration management processes and tools for future systems.

Additionally, Ben continued his annual effort to assist an ALCF-sponsored team in SC's Student Cluster Competition, providing logistical, setup, and application support to the Chicago Fusion team at SC17.

Edouard Brooks
Software Developer

Edouard got his start at the ALCF as part of the facility's summer student program in 2016, with a project focused on testing the capabilities of commercial virtual reality (VR) platforms for scientific visualization. One of his efforts involved using VR technologies to explore mouse brain datasets from an ALCF Data Science Program project aimed at understanding brain structure and pathology.

After graduating with a bachelor's degree in computer science from the University of Chicago, Edouard joined the ALCF full time in 2017. He continues his work to develop VR software to help researchers engage with their 3D datasets in more intuitive ways than afforded by traditional 2D approaches. For example, Edouard is investigating immersive VR techniques to demonstrate its benefits for data analysis, including mobility (i.e., the ability to walk around and through datasets) and interactivity (i.e., the ability to manipulate and explore data by hand). In addition to helping ALCF users explore innovative visualization methods, Edouard has presented his work with immersive VR as a guest lecturer for introductory VR courses at the School of the Art Institute of Chicago.

Yasaman Ghadar
Postdoctoral Researcher

A computational chemist by training, Yasi collaborates on cross-divisional projects at Argonne that utilize molecular dynamics simulations to elucidate the structural properties of complex chemical and physical systems, such as lithium-ion batteries and semiconductors.

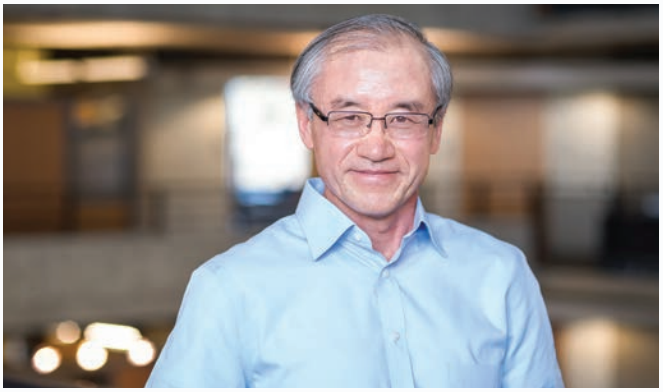
She is also investigating the capabilities, performance, and scalability of simulation, data, and machine learning approaches for current and future HPC platforms. Her work in this area includes a project at Argonne's Joint Laboratory for System Evaluation aimed at understanding the performance of different machine learning frameworks.

In addition to her day-to-day work, Yasi has made it a priority to participate in outreach and mentoring activities across the laboratory. In 2017, she served as the chair of the Argonne Postdoctoral Society Symposium, an annual event that allows postdocs and students to showcase their work and helps them to prepare for the next phase of their careers. Yasi also mentored ALCF summer students on two separate projects this year: one effort involved coupling the graph analytics package ChemNetwork into the LAMMPS molecular simulation code to enable in-situ analysis; and the other project focused on investigating ion solvation in battery electrolytes.

Elise Jennings
Computer Scientist

With expertise in machine learning and advanced statistical methods, Elise is helping the ALCF support a growing number of projects in the data and learning space. Since joining the ALCF in April, she has been working with project teams to apply these analytical techniques to gain insights into large scientific datasets produced by experimental, simulation, or observational methods. For example, she is working with researchers from GE Global Research on an ALCF Data Science Program project that is using machine learning and datasets from large-eddy simulations to develop improved turbulence models.

With a PhD in cosmology and previous experience as a research associate in Fermilab's Theoretical Astrophysics Group, Elise drew on her background to deliver a brief lecture on historical efforts to study the solar eclipse, as a master of ceremony at Argonne's Eclipse Fest in August. She has been very active in other Argonne outreach activities as well, serving as a career advice panelist and poster symposium judge for postdocs, and volunteering for students events, like Introduce a Girl to Engineering Day, Hour of Code, and Science Bowl.



Álvaro Vázquez-Mayagoitia
Computational Scientist

An expert in computational and theoretical chemistry, Álvaro works closely with project teams to help them achieve their science goals by maximizing their use of ALCF computing resources. With broad experience implementing electronic structure theory applications and methods on HPC systems, he has been driving the continued enhancement of notable quantum chemistry codes, including NWChem, MADNESS, and FHI-aims.

In addition to supporting teams participating in INCITE and ALCC projects, Álvaro is collaborating with two projects in the ALCF Data Science Program that are deploying machine learning approaches and complex workflows to accelerate materials discovery. His work with these projects has contributed to advancements in predicting organic dyes to improve solar cells, and in the study of inner forces of molecular crystals with applications in medicine and electronics.

Álvaro also leads the ALCF Postdoctoral Committee, where he manages the recruitment and hiring of postdoctoral researchers to work on both computational science projects and software development efforts for next-generation supercomputers. As part of this role, he is actively involved in mentoring ALCF postdocs to ensure they are developing the skills and experience needed to advance their careers.

Michael Zhang
Software Developer

Michael supports the ALCF's business intelligence efforts by designing and implementing automated tools that assimilate and verify data from several different systems at the facility. His responsibilities include developing extraction, transformation, and load (ETL) programs; data mining models; and business reports.

In 2017, Michael built an ETL program to bring Theta system, maintenance, and usage data into the facility's centralized database, known as the Data Warehouse. Designed to capture precise results at the machine's node level, the Theta ETL automatically collects data on system change events, such as job failures, which staff members can use to identify and resolve performance-related issues. In addition to providing insights into how Theta is operating, Michael's program produced data for various ALCF reports, including the annual Operational Assessment Review.

Michael also created and launched the ALCF Publication Discovery Program in 2017. This automated system searches the Crossref website (www.crossref.org) for academic research articles published by ALCF users. Ultimately, Michael's efforts are helping to improve the efficiency and accuracy of data collection, maintenance, analysis, and reporting at the ALCF.

ALCF Computing Resources

The ALCF provides users with access to supercomputing resources that are 10 to 100 times more powerful than systems typically used for 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. Billions of computing hours are allocated on ALCF systems each year.

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

Theta

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

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

Cetus

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

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

Iota

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

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

Vesta

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

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

Cooley

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

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

Supporting Resources

Data Storage

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

DISK STORAGE

The Mira system consists of 384 I/O nodes that connect to 22 storage arrays that control 13,000 disk drives with a total useable capacity of 27 PB and a maximum aggregate transfer speed of 330 GB/s over two file systems. Mira uses the General Parallel File System (GPFS) to access the storage. The Theta system consists of 30 I/O nodes that connect to a storage array that controls 2,300 disk drives with a total useable capacity of 9 PB and a maximum aggregate transfer speed of 240 GB/s. Theta uses Lustre to access this storage.

TAPE STORAGE

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

Networking

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

The ALCF connects to other research institutions using up to 100 Gb/s of network connectivity. Scientists can transfer datasets to and from other institutions over fast research networks, such as ESnet and Internet2.

Testbeds

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

Intel Xeon Phi Knights Landing Cluster	**AppliedMicro X-C1 Server Development Kit Plus**
Cray Urika-GX Analytics Platform	**NVIDIA DGX–1**
IBM Power System S822LC	**IBM Elastic Storage Server GL6**

Enabling Science with HPC Services and Tools

The ALCF deploys several innovative computing services and software tools that are critical to enabling efficient facility operations and boosting scientific productivity among facility users.

Leading-edge supercomputers like Mira and Theta are one-of-a-kind machines designed to serve the needs of the scientific computing community.

Operating these unique computing resources requires specialized software, tools, and services to ensure users and administrators can get the most out of the system's vast capabilities.

At the ALCF, staff members develop and operate custom-built software tools designed for specific tasks, as well as open-source software tools adapted to meet various facility needs. These tools help ensure scientific applications run efficiently on its leadership-class systems, and generate data that guides future support and research priorities.

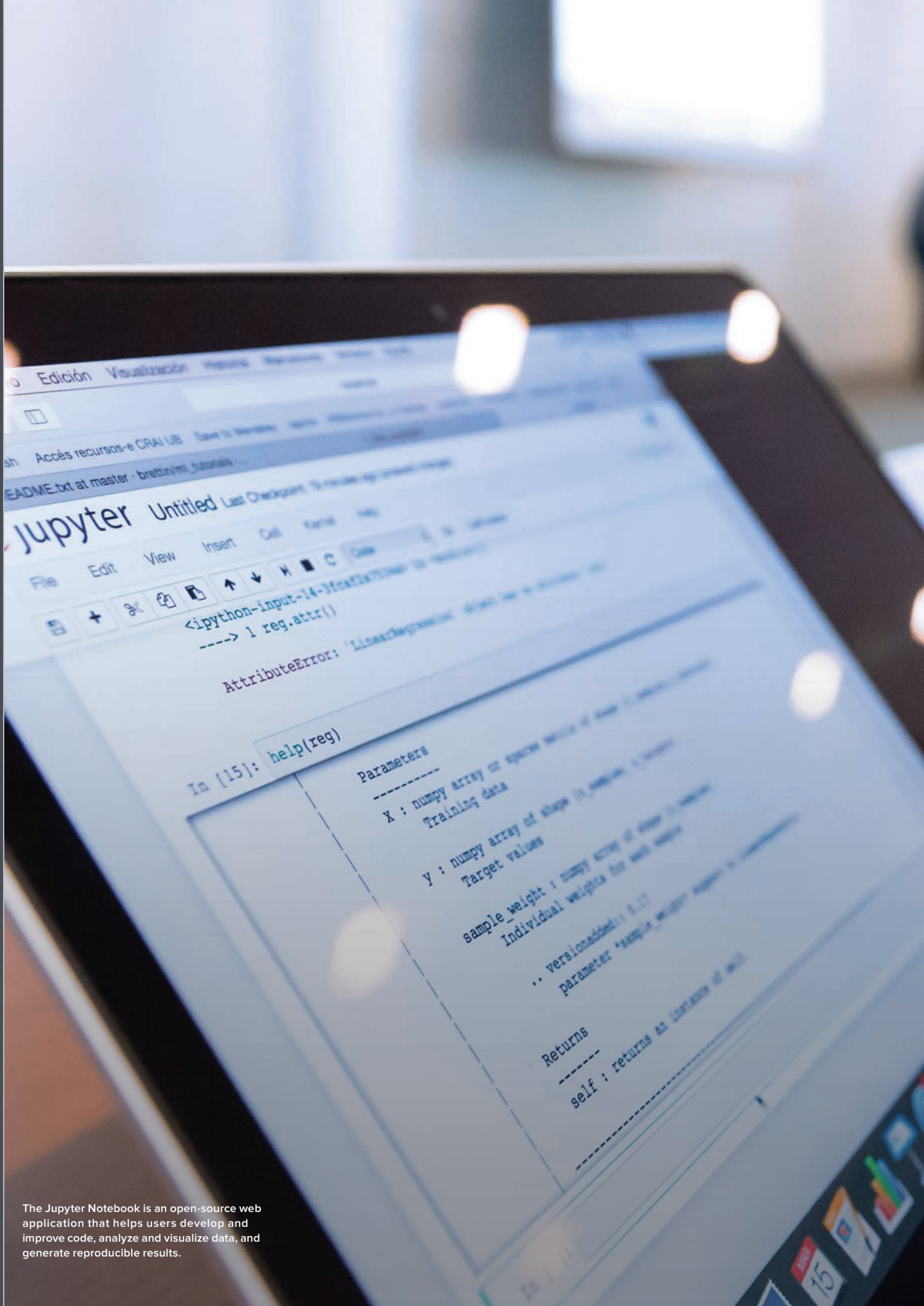
For example, in 2017, the facility launched a new web application called Audience that allows staff members to closely monitor file system traffic and performance.

In an effort to expand its scope beyond that of a traditional HPC facility, the ALCF has also begun to introduce services that will help improve collaboration among research teams, eliminate barriers to productively using the facility's systems, and integrate with user workflows to produce seamless, usable environments.

In 2017, the facility deployed two new services—Jupyter Notebook and HTCondor-CE—to enable advances among current projects and encourage new disciplines to leverage ALCF resources to accelerate their research.

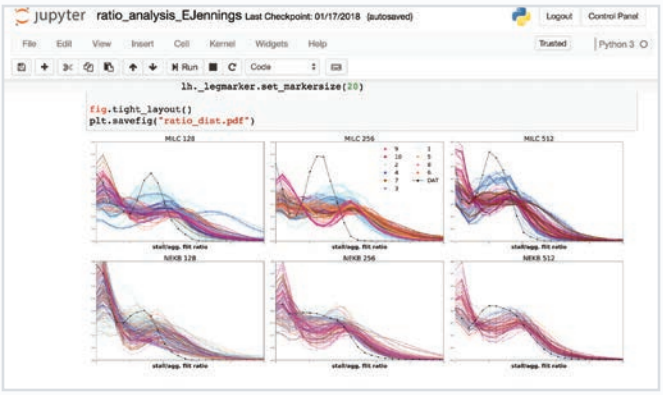
With the ability to create and share documents containing code and visualizations, the Jupyter Notebook service is providing staff members and users with a highly collaborative tool that is helping to enhance code development, data analysis, visualizations, and more. At the SC17 conference, Argonne researchers demonstrated how Jupyter Notebooks can be used to build a service for interactive, scalable, and reproducible data science.

HTCondor-CE was first deployed as part of a collaborative project with CERN's Large Hadron Collider. For large-scale experiments and other projects with complex workflow, this "gateway" software tool simplifies the integration of ALCF resources, making it easier for users to submit jobs from outside the facility.



The Jupyter Notebook is an open-source web application that helps users develop and improve code, analyze and visualize data, and generate reproducible results.

Services



The ALCF deployed the Jupyter Notebook service to provide researchers with a collaborative tool for code development, data analysis, and educational purposes.

Jupyter Notebook

OVERVIEW Jupyter Notebook is an open-source web application that allows users to create and share documents containing code, visualizations, and text. In 2017, the ALCF deployed a proof-of-concept Jupyter service that provides users with a notebook and access to Mira's filesystems for data analysis. The service also offers limited job submissions to the ALCF's visualization cluster, Cooley, through Jupyter's terminal interface.

FEATURES This interactive tool allows users to capture the process of developing, documenting, and executing code in more than 40 different programming languages.

Users can provide edits and commentary to documents using a Markdown parser that is TeX and LaTeX-aware. Jupyter Notebook can be integrated with other HPC tools to help users analyze massive datasets and produce visualizations of the results. JupyterHub, a multi-user version of the notebook, gives users a shared project space for collaborative research.

BENEFIT Jupyter Notebook provides a highly collaborative tool for developing and improving code, analyzing and visualizing data, and generating reproducible results. It gives users the ability to work with a variety of frameworks in an interactive environment (e.g., Apache Spark for data-intensive jobs; TensorFlow or Keras for machine/deep learning and visualization; and advanced statistics packages or libraries for other research needs). In addition, Jupyter is a valuable tool for educational purposes, enabling researchers to develop teaching materials for students, workshops, and other training-related activities.

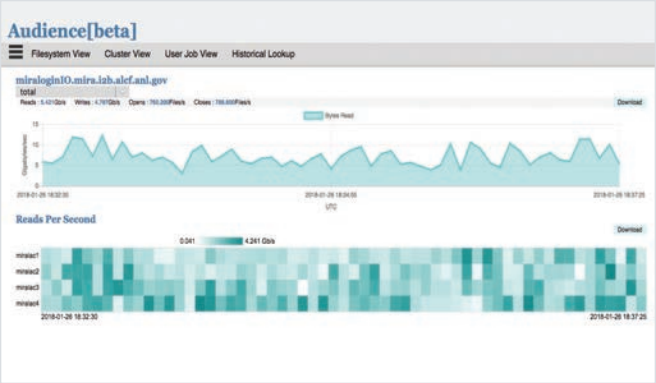
HTCondor-CE

OVERVIEW HTCondor-CE is a "gateway" software tool developed by the Open Science Grid to authorize remote users and provide a resource provisioning service. In 2017, ALCF staff deployed a pilot of HTCondor-CE for Mira and Cooley, with plans to extend the service to Theta next year. This effort requires writing code to allow HTCondor-CE to interact with the ALCF's Cobalt job scheduler, as well as making modifications to the facility's authentication policy.

FEATURES The HTCondor-CE allows authenticated users to submit jobs remotely to ALCF systems without establishing an interactive shell login.

BENEFIT For projects with complex workflows, this tool helps simplify the integration of ALCF resources as production compute endpoints. Using HTCondor-CE, research teams benefit from the ability to carry out multiple computing steps at one facility. In 2017, researchers from an ALCF Data Science Program project, involving the Large Hadron Collider's ATLAS experiment, performed initial pilot testing of HTCondor-CE on Cooley with the goal of integrating the tool with the ATLAS project's internal workflow management system.

Software Tools



The Audience web application was developed to help staff members monitor file system traffic and performance on ALCF resources.

Audience

OVERVIEW Audience is an ALCF-developed web application designed to monitor file system traffic and performance.

FEATURES The tool presents reads/writes per second and file opens/closes per second in graphical form for live and historical GPFS cluster performance. Audience is also able to provide live and historical performance data at a job level without impeding an application.

BENEFIT By providing a visual representation of file system performance, Audience helps ALCF staff members troubleshoot system-related issues and identify issues that could help improve the performance of user applications.

AutoPerf

OVERVIEW AutoPerf is an ALCF-developed library that automatically collects performance information for applications running on ALCF systems.

FEATURES This tool records data from simulations and saves it for analysis when the job is completed. Output includes MPI usage and performance information that indicates which MPI routines were called, how many times each routine was called, the time spent in each routine, the number of bytes sent or received (if applicable), and data from the system's hardware performance counters.

BENEFIT AutoPerf data helps ALCF staff better understand the requirements of applications and how to optimize their performance. In addition, AutoPerf data recently has been used to evaluate the impact of injection bandwidth on applications and to inform the development of future ALCF systems.

Business Intelligence Tools

OVERVIEW The ALCF's Business Intelligence (BI) team has developed automated systems to assimilate and verify data from many ALCF systems to ensure the accurate reporting of facility information to users, ALCF leadership, and DOE.

FEATURES The automated systems continuously extract data from several disjointed systems at the facility and convert the data into dimension and fact tables with a standard set of units. The data are loaded into a centralized database, known as the Data Warehouse. Additional processing combines multiple datasets into smaller datasets suitable for use by the BI team's reporting software. The team has automated tools in place to ensure the accuracy and completeness of all data pulled from the Data Warehouse.

BENEFIT The ALCF's BI tools have greatly improved the efficiency of data collection, maintenance, analysis, and reporting at the ALCF.

A web-based tool called the Gronkulator pulls machine status information from Colbalt to provide users and staff with a real-time look at ALCF system activity.

Cobalt

OVERVIEW Cobalt is the ALCF's job scheduler and resource manager.

FEATURES Cobalt gives users the ability to set up and run various workloads on all ALCF systems, including interactive mode jobs and batch scripts. It allows users to specify common tasks in a system-agnostic fashion, while offering more fine-grained control of job submissions for users seeking to leverage advanced features of ALCF systems. Cobalt also handles placement of user tasks on ALCF resources, optimizing use of these systems, as well as exposing advanced system features to users and their workloads. In 2017, the ALCF enabled per-job on-demand node rebooting with Cobalt on Theta, allowing users to request the optimal memory mode configuration for their workload. The scheduler was also upgraded to take these requests into account and minimize the cost of requested reboots, while maintaining throughput and turnaround times for users.

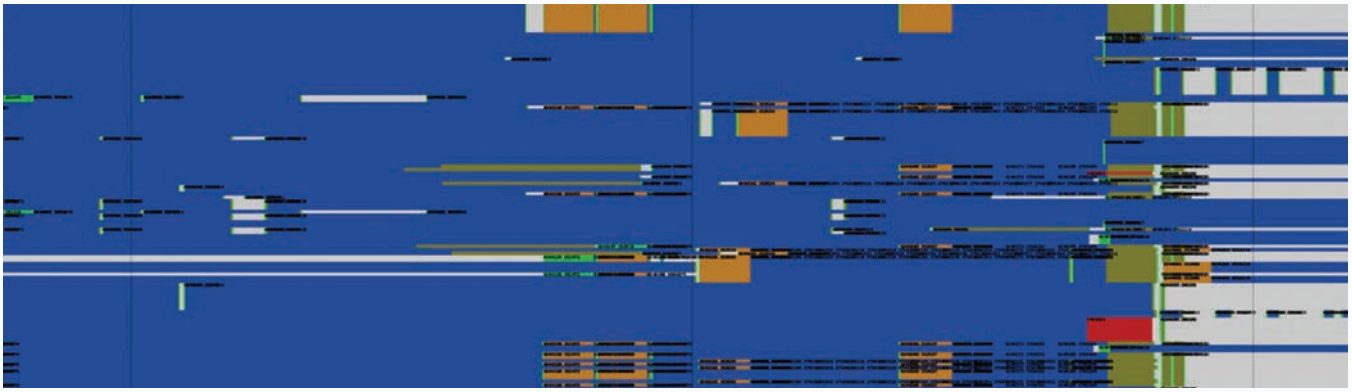
BENEFIT This tool gives the ALCF great flexibility in executing its scheduling policies, accommodates diverse workloads, and supports important features (e.g., alternate kernel support, per-job arbitrary memory mode selection) that are either not supported or poorly supported by other schedulers and resource managers.

Library Tracking

OVERVIEW The ALCF uses software tools to track the usage of various libraries on its systems. The ALCF developed the TrackLib and Trackdeps tools to perform this task on Mira. For Theta, the ALCF has deployed the Trackdeps and the XALT library tracking system, which has been in use on Cray systems for many years, and customized it to meet the specific needs of the facility.

FEATURES Trackdeps records paths to all build process inputs that contribute to the final output, including compiler identity, header files, Fortran module files, and libraries. Tracklib examines programs as they run on Mira, producing the data necessary to match the job's accounting information with the data collected by Trackdeps. XALT tracks executable information and linkage of static shared and dynamically linked libraries. The data collected by these tools are extracted and imported into the ALCF's Data Warehouse. A single interface for interrogating data from both Mira and Theta is under development, and is expected to be available in 2018.

BENEFIT With these tools in place, staff can determine how various libraries are being used at the facility, providing knowledge that not only helps to prioritize library development and maintenance efforts, but also proves useful when planning future systems.



The ALCF's Job Failure Analysis system provides staff members with a visual representation of user jobs, system reservations, node availability, and more.

Darshan

OVERVIEW ALCF researchers are collaborating with staff from Argonne's Mathematics and Computer Science Division on the continued development of Darshan, a scalable HPC I/O instrumentation library designed to capture an accurate picture of application I/O behavior.

FEATURES Darshan records statistics such as the number of files opened, time spent performing I/O, and the amount of data accessed by an application. The tool's lightweight design makes it suitable for full-time deployment for workload characterization of large systems. Darshan is portable across a wide variety of platforms and is now deployed at multiple DOE computing facilities.

BENEFIT At the ALCF, Darshan is available to both users and administrators to aid in performance tuning and debugging of scientific applications. Darshan also serves as a foundational component of multiple forward-looking computer science research projects, including the Total Knowledge of I/O (TOKIO) project, a DOE-funded collaboration between Argonne and Lawrence Berkeley National Laboratory that seeks to combine many instrumentation sources into a holistic view of I/O performance; and a SciDAC project that is applying statistical modeling techniques to better understand performance variability and the correlation between application and system performance.

Job Failure Analysis

OVERVIEW The ALCF developed a software system to help staff members assess all failed jobs that occur on the facility's computing systems.

FEATURES The system allows interactive querying of job data and annotation of job status. It saves job data in real time to the ALCF's Operational Data Processing Service (ODPS), a database that allows staff to track usage, availability, reservations, jobs, or any event that happens over time using an ALCF computing resource. ODPS was developed to be highly scalable for use on the facility's next-generation systems.

BENEFIT The ALCF's job failure analysis system helps staff members resolve system-related issues and identify issues that could help improve user productivity.

sbank

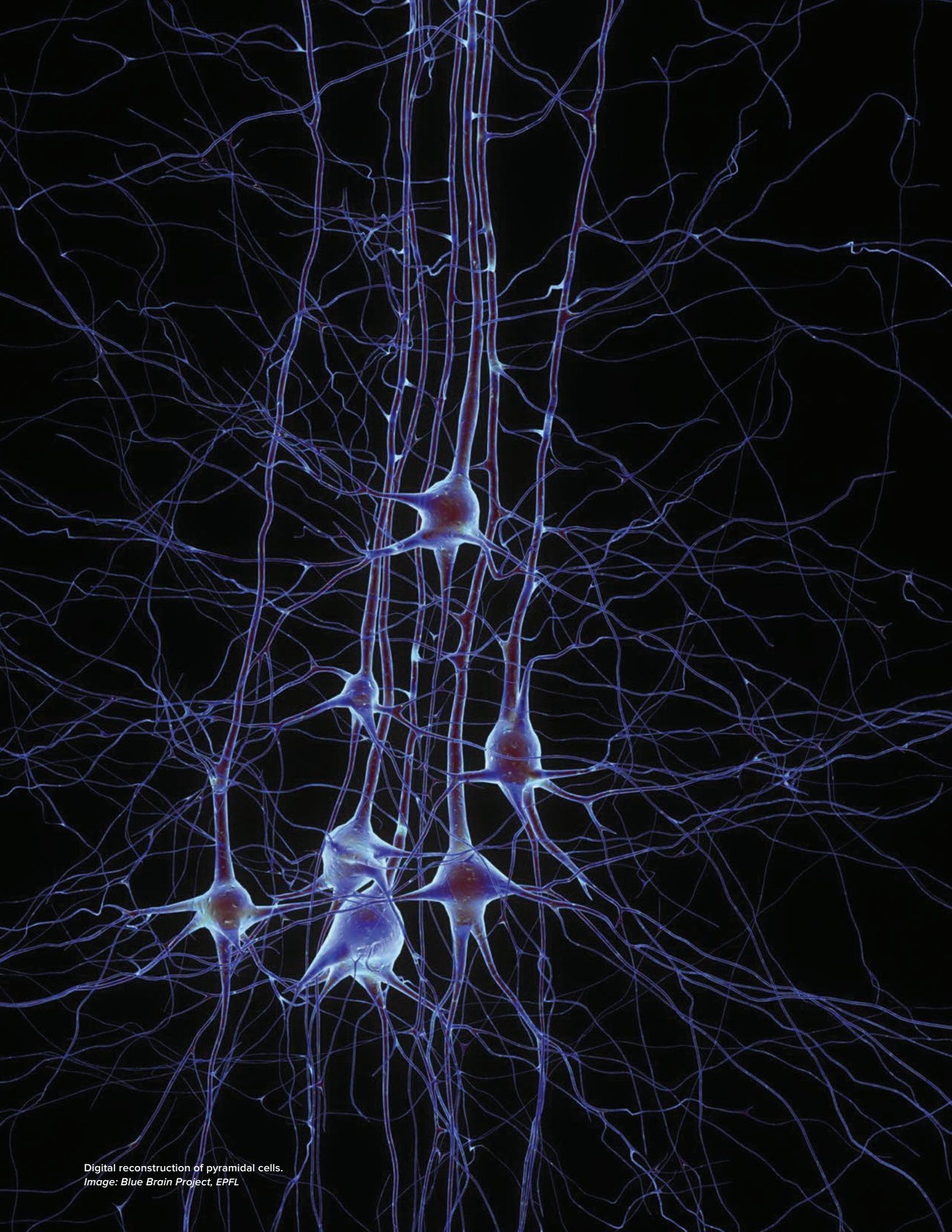
OVERVIEW sbank is the ALCF's job accounting system.

FEATURES This customized software system, which processes output from the Cobalt scheduler, is designed to allow users to track project allocations, usage charges, and refunds. It gives users the ability to query the balance and expiration of their project.

BENEFIT This tool enables users to monitor and manage their allocation usage by user, job, and computing system.

SCIENCE

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



Digital reconstruction of pyramidal cells.
Image: Blue Brain Project, EPFL

Accessing ALCF Resources for Science

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

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

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

Application Programs

ADSP

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

ESP

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

Allocation Programs

INCITE

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

ALCC

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

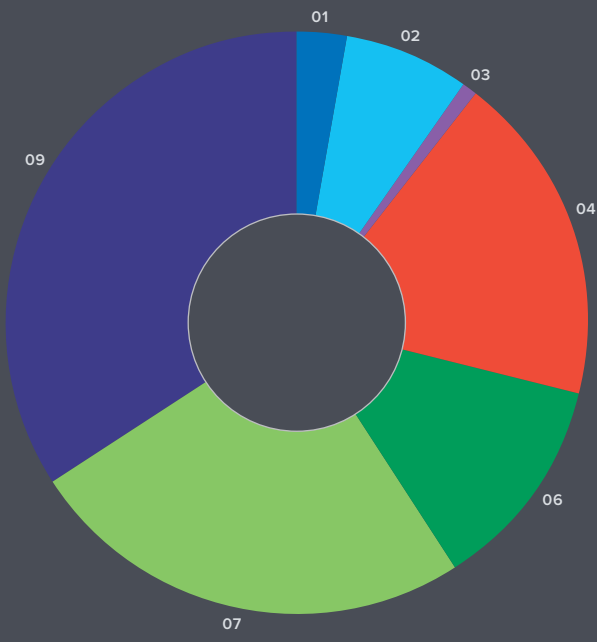
DD

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

INCITE/ALCC BY DOMAIN

2017 INCITE
3.53 Billion Core-Hours

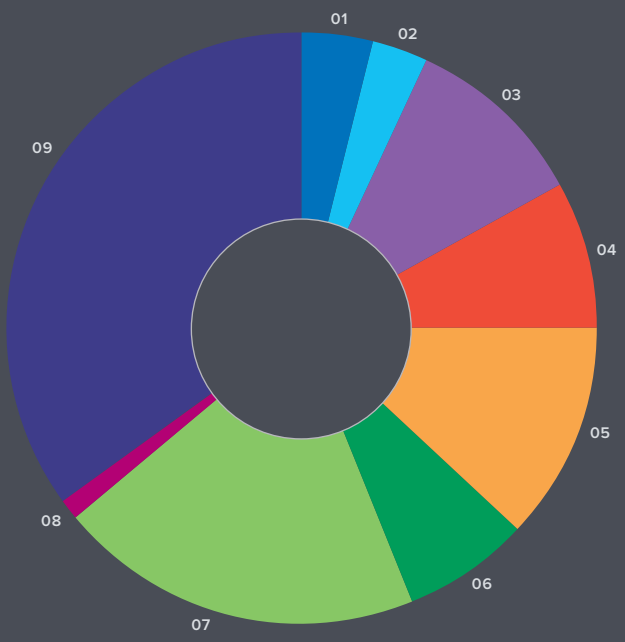
01	Biological Sciences	3%
02	Chemistry	7%
03	Computer Science	1%
04	Earth Science	18%
05	Energy Technologies	-
06	Engineering	13%
07	Materials Science	25%
08	Mathematics	-
09	Physics	33%



2017 ALCC
1.97 Billion Core-Hours

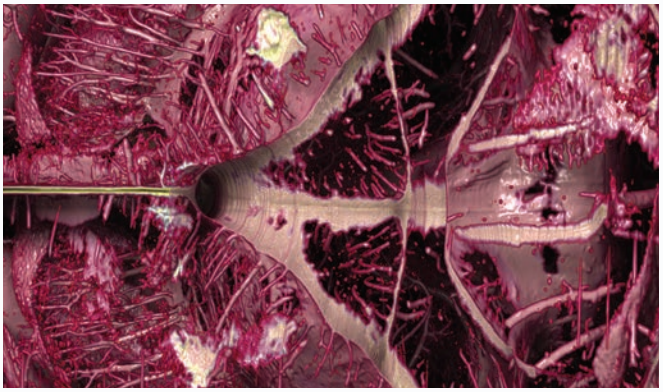
01	Biological Sciences	4%
02	Chemistry	3%
03	Computer Science	10%
04	Earth Science	8%
05	Energy Technologies	12%
06	Engineering	7%
07	Materials Science	20%
08	Mathematics	1%
09	Physics	35%

Note: ALCC data are from calendar year 2017.



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

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



Reconstructed cerebrovascular network of a mouse brain using synchrotron microtomography. *Image: Joseph A. Insley, Argonne National Laboratory*

CHALLENGE Through the ALCF Data Science Program, this project is developing a large-scale data and computational pipeline that integrates exascale computational approaches for understanding brain structure and pathology. Initial studies will focus on the reconstruction of mice brains utilizing novel imaging and analytical tools to image, for the first time, at the level of individual cells and blood vessels.

APPROACH The team will use X-ray microtomography, a high-resolution 3D imaging technique, to analyze the brain of a petite shrewmouse at submicron resolutions, providing a detailed picture of blood vessels and cell bodies. An electron microscope then will allow for the capture of all the synaptic connections between individual neurons at small targeted regions guided by the X-ray microtomography. Data provided by these images will require the development of reconstruction, segmentation, and analysis tools, and their seamless integration onto large-scale computing systems. To meet this goal, researchers currently are focused on tweaking their codebase on advanced Intel architectures.

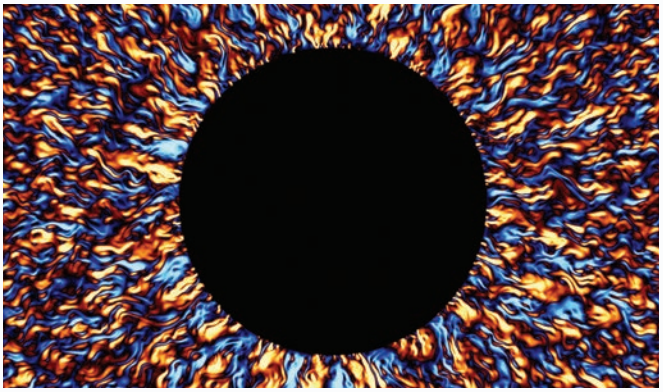
In addition, the team is introducing scalable workflows focused on analysis and visualization of experimental data, such as the RhoAna framework, a machine learning-based technique. These combined techniques will, for the first time, allow researchers to compare potential organizational patterns across brains to determine which are genetic and which are unique.

RESULTS Using an MPI-based master/worker model, the team ran existing codebases effectively on the ALCF's Cooley system. The researchers developed benchmarking tools to evaluate the performance of these applications. Their benchmarking efforts have focused on making it easy to rapidly explore combinatoric build and run options, while automating analysis. This led to the packaging of code for use in the Spack package manager framework.

IMPACT This research will help provide a clearer understanding of how even the smallest changes to the brain play a role in the onset and evolution of neurological diseases, such as Alzheimer's and autism, and perhaps lead to improved treatments or even a cure.

Frontiers in Planetary and Stellar Magnetism Through High-Performance Computing

PI Jonathan Aurnou
INST University of California, Los Angeles
HOURS INCITE, 260 Million Core-Hours



Radial velocity field (red = positive; blue = negative) on the equatorial plane of a numerical simulation of Earth's core dynamo. These small-scale convective flows generate a strong planetary-scale magnetic field. *Image: Rakesh Yadav, Harvard University*

CHALLENGE Magnetic fields are generated deep in the cores of planets and stars by a process known as dynamo action. This phenomenon occurs when the rotating, convective motion of electrically conducting fluids converts kinetic energy into magnetic energy. To better understand the dynamics that lead to magnetic field generation, a research team is using ALCF computing resources to simulate the turbulent interiors of Earth, Jupiter, and the Sun at an unprecedented level of detail.

APPROACH With this multiyear INCITE project, researchers are developing high-resolution 3D models of planetary and stellar dynamo action in turbulent fluids with realistic material properties. Working with ALCF staff, the team has optimized Rayleigh, an open-source code designed to study magnetohydrodynamic (MHD) convection in spherical geometries, for Mira, allowing them to resolve a range of spatial scales previously inaccessible to numerical simulation.

RESULTS The team successfully implemented rotation into their solar dynamo model, which led to some of the highest-resolution and most turbulent simulations of solar convection ever performed. In a paper published in *The Astrophysical Journal Letters*, the team discussed how they used the simulations to place upper bounds on the typical flow speed in the solar convection zone—a key parameter to understanding how the Sun generates its magnetic field and transports heat from its deep interior. In addition, the researchers have made significant progress with their Jupiter convection zone model, enabling the highest-resolution giant-planet simulations yet achieved. The Jupiter simulations will be used to make detailed predictions of surface vortices, zonal jet flows, and thermal emissions that will be compared to data from NASA's Juno mission. Finally, ongoing simulations of Earth's geodynamo are showing that flows and coupled magnetic structures develop on both small and large scales, revealing new MHD processes that do not appear to develop in low-resolution computations.

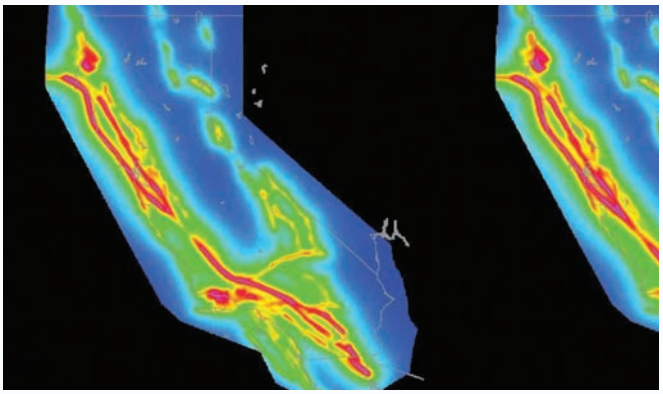
IMPACT This project is developing advanced dynamo models to shed light on the interplay of magnetism, rotation, and turbulent convection occurring within the remote interiors of planets and stars. The resulting datasets, which will be made publicly available to the broader research community, will help advance the understanding of dynamo processes and provide new insights into the birth and evolution of the solar system.

PUBLICATIONS

Featherstone, Nicholas A., and Bradley W. Hindman. "The Emergence of Solar Supergranulation as a Natural Consequence of Rotationally Constrained Interior Convection." *The Astrophysical Journal Letters 830, no. 1* (October 2016), American Astronomical Society.

Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations

PI Thomas H. Jordan
INST University of Southern California
HOURS INCITE, 141 Million Core-Hours
ALCF: 45M; OLCF: 96M



California seismic hazard map generated with the physics-based RSQSim and empirical UCERF3 models. Maps show the peak ground acceleration, plotted in units of surface gravity, expected with two percent probability of exceedance in 50 years. *Image: Kevin Milner, University of Southern California*

CHALLENGE Human and economic risks in seismically active regions continue to increase as urban areas and their dependence on interconnected infrastructure networks continue to grow. Understanding seismic hazards across a wide spectrum of forecasting and response times, including a proper assessment of modeling uncertainties, is the foundation on which most seismic risk-reduction strategies are developed. The Southern California Earthquake Center (SCEC) is using DOE resources to improve the accuracy of earthquake simulations to better understand seismic hazard and assess seismic risk.

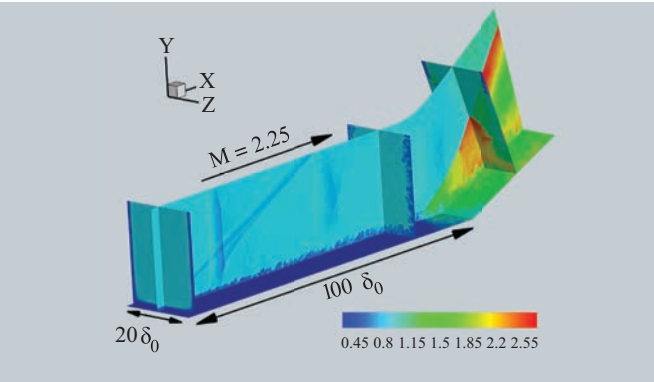
APPROACH The team used Mira to run the earthquake simulator code RSQSim, which produces long-term synthetic earthquake catalogs. A baseline simulator model was developed with several global uniform model parameters tuned to match earthquake scaling observations. The researchers also turned to Mira to run the new dynamic rupture simulation code, Waveqlab3D, which requires relatively few points per wavelength, allowing for both physics-based spontaneous dynamic rupture as well as wave-propagation for ground motion prediction. This eliminates the need for a two-step approach, simplifying the workflow in addition to reducing data storage.

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

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

Direct Numerical Simulation of Compressible, Turbulent Flow

PI Jonathan Poggie
INST Purdue University
HOURS INCITE, 200 Million Core-Hours



Overview of the instantaneous density field in a compression ramp interaction with resolved sidewall boundary layers. The grid consisted of 9.4 billion cells and was run on Mira using 524,288 cores (65,536 MPI ranks with eight OpenMP threads per rank). *Image: Jonathan Poggie and Kevin M. Porter, Purdue University*

CHALLENGE Much progress has been made toward routine flight at higher speeds, but the presence of intense, unsteady aerodynamic loads remains a fundamental design difficulty. Large-scale, low-frequency pressure fluctuations that occur in the presence of flow separation can lead to severe structural fatigue loading, shorter lifespan, and even catastrophic failure. The reason for such low-frequency oscillations in the separated flow remains an open scientific question.

APPROACH This project aims to settle the long-standing question of amplifier versus oscillator, the two conceptual models of separation unsteadiness. In the oscillator model, the separated flow has an inherent instability, which leads to self-excited oscillations. No inputs are required, because any small fluctuations in the amplified frequency range are reinforced through positive feedback. In the amplifier model, disturbances in the incoming flow are selectively amplified in the separated flow. The separation region has a characteristic space and time scale, and it reacts strongly to disturbances on the order of these scales, but not to smaller-scale disturbances.

To test the amplifier and oscillator models, computations must capture both incoming turbulence and separation bubble motion. Because of the large range of scales between fine-grained turbulence and separation bubble motion, this research requires large calculations that will run on long time scales. To this end, the researchers have developed an adaptive, compact-difference code that can capture both fine-grained turbulence and shock waves. Multilevel parallelism in the code structure enables very fast execution on Mira.

RESULTS In an earlier phase of this project, researchers carried out the first-ever fully resolved computation of a shock-wave/boundary-layer interaction, enabling them to study the interaction of the shock with turbulence-generated sound. This has led to the present study of an analogous case with a laminar inflow, and the search for evidence of large-scale separation bubble motion in the absence of incoming disturbances. The team is also exploring flow control, that is, the effects on the separation bubble of controlled disturbances in the incoming flow.

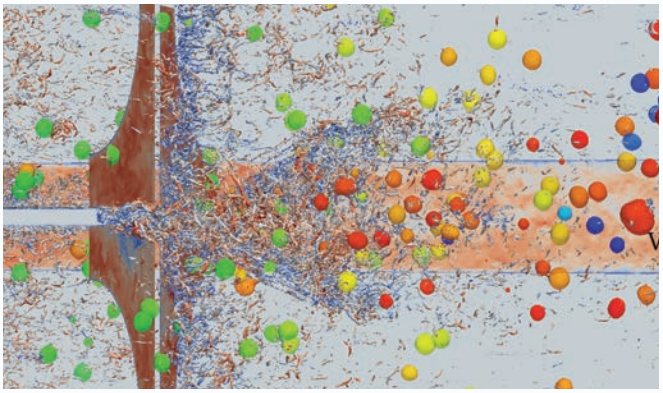
IMPACT Numerical simulations are revealing the origin of the separation unsteadiness that drives fatigue loading on high-speed aircraft. With this new understanding of the flow physics, researchers are exploring flow modification and control to enable a new generation of fast, reliable aircraft.

PUBLICATIONS

Porter, Kevin M., and Jonathan Poggie. "Turbulence Structure and Large-Scale Unsteadiness in Shock-Wave/Boundary Layer Interaction," *55th AIAA Aerospace Sciences Meeting* (January 2017).

Multiphase Simulations of Nuclear Reactor Flows

PI Igor Bolotnov
INST North Carolina State University
HOURS ALCC, 72.1 Million Core-Hours



Direct numerical simulation of turbulent flow in a nuclear reactor subchannel with fully resolved internal structures. *Image: Jun Fang, Argonne National Laboratory*

CHALLENGE Boiling phenomena, bubble formation, and two-phase (liquid/gas) flow in nuclear reactor geometries are important physical processes that affect nuclear reactor safety. In particular, high-bubble concentrations in pressurized water reactor (PWR) designs can lead to a phenomenon called departure from nucleate boiling and cause overheating and disintegration of the fuel if the fluid conditions are not designed properly. This project seeks to gain a deeper understanding of boiling phenomena, bubble formation, and two-phase flow in nuclear reactor geometries through direct numerical simulation of fully resolved, deformable bubbles at unprecedented scale.

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

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

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

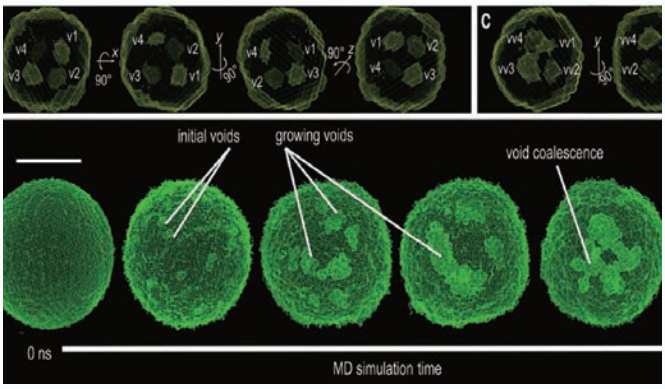
IMPACT The improved boiling phenomena models directly contribute to CASL's mission of developing advanced modeling and simulation tools to improve the operation and safety of the existing nuclear fleet. These efforts are essential in transitioning the historically conservative nuclear industry to adopt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

PUBLICATIONS

Fang, Jun, Michel Rasquin, and Igor A. Bolotnov. "Interface Tracking Simulations of Bubbly Flows in PWR Relevant Geometries," *Nuclear Engineering and Design* (February 2017), Elsevier.

Atomistic Simulations of Nanoscale Oxides and Oxide Interfaces

PI Subramanian Sankaranarayanan
INST Argonne National Laboratory
HOURS ALCC, 120 Million Core-Hours



Snapshots of the 3D structure of iron nanoparticles in the course of the oxidation process, captured through large-scale reactive molecular dynamic simulations. *Image: Ganesh Kamath, Badri Narayanan, Sheng Peng, Subramanian Sankaranarayanan, and Xiaobing Zuo, Argonne National Laboratory; Yugang Sun, Temple University*

CHALLENGE When metals oxidize, there is a directional flow of material across an interface, which can lead to the formation of holes in the atomic lattice. These holes can take the form of rusted-out metal, or, if carefully controlled, of exotic structures, such as hollowed-out nanoparticles or nanoshells. These unique structures have been used as electrodes in battery applications and as vehicles for drug delivery in medicine. The key to creating useful structures lies in controlling the shape, structure, and distribution of the holes. Controlling these variables requires a deep understanding of the oxidation process and its progression in time. Researchers from Argonne and Temple University used Mira's immense computing power to simulate oxidation of iron nanoparticles and watch them in real time as they oxidized.

APPROACH Armed with information obtained from small-and wide-angle X-ray scattering, the team integrated these observations with large-scale reactive molecular dynamics simulations. To perform these simulations, the team collaborated with ALCF staff to optimze the LAMMPS molecular dynamics program for Mira. Focusing on oxidation of small particles of iron at the nanoscale level, specifically in the 10-nanometer range, they observed and modeled the changes in nanoparticle geometry as they occurred.

RESULTS The research team tracked the full 3D geometrical evolution of the transformation of unstructured iron nanoparticles into crystalline iron hollow nanoshells, and confirmed experimental observations with the dynamical simulations performed on Mira. Their work furthered understanding of the atomic-level mechanisms underlying the geometrical transformation and highlighted how the oxidation process has parameters that can be tuned. The effort demonstrated that the methodology used in this study, which enabled quantitative reconstruction of the 3D geometry of the nanoparticles, has the potential to address many fundamental questions in materials science and chemistry.

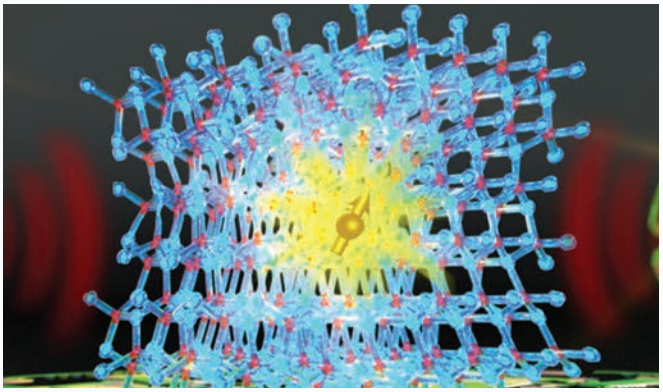
IMPACT This project is developing advanced understanding of the chemical reaction that transforms iron nanoparticles into nanoshells. Nanoshells have already functioned as vehicles in drug delivery and battery technologies. Learning how to better control such reactions at the atomic level will advance these applications.

PUBLICATIONS

Sun, Y., X. Zuo, S. K. R. S. Sankaranarayanan, S. Peng, B. Narayanan, and G. Kamath. "Quantitative 3D Evolution of Colloidal Nanoparticle Oxidation in Solution," *Science* (April 2017), AAAS.

Computational Engineering of Defects in Materials for Energy and Quantum Information Applications

PI Marco Govoni
INST The University of Chicago and Argonne National Laboratory
HOURS ALCC, 53.7 Million Core-Hours



This figure illustrates the spin of a nitrogen vacancy in aluminum nitride designed for quantum bit applications. *Image: Hosung Seo, The University of Chicago; Giulia Galli and Marco Govoni, The University of Chicago and Argonne National Laboratory*

CHALLENGE Defects in materials can have unexpected and peculiar properties that may degrade a material's performance. However, the unusual properties of defects can be used to design new functionalities that are not present in their host materials. With this ALCC project, researchers are developing a first-principles theoretical framework to study the properties of defects in soft and hard matter. This will enable the investigation of new materials for applications, including solar-powered fuel production from water and solid-state quantum computing and sensing.

APPROACH The team's computational framework is based on *ab initio* molecular dynamics and accurate electronic structure simulations using the open-source Qbox, Quantum Espresso, and WEST codes. Optimized to run on Mira, these scalable, integrated first-principles codes are capable of tackling systems of unprecedented size (several thousands of electrons) that are crucial to simulating realistic liquid electrolytes and isolated atom-like defects in bulk crystals. The researchers are using the framework to obtain atomic trajectories; compute thermodynamic and electronic properties of electrolytes; and perform high-throughput calculations to identify new potential spin quantum bits (qubits) in semiconductors, such as silicon carbide and aluminum nitride.

RESULTS In a paper published in *Science Advances*, the team demonstrated its efficient and accurate approach for predicting the electronic properties of aqueous solutions. The researchers studied the photoelectron spectra of a broad range of solvated ions, showing that first-principles molecular dynamics simulations and electronic structure calculations using dielectric hybrid functionals provide a quantitative description of the electronic properties of the solvent and solutes, including excitation energies. Their theoretical results were validated through comparison to data from state-of-the-art photoelectron liquid-jet experiments. In addition, the team published a paper in *Physical Review X*, detailing their development of a generalization of dielectric hybrid functionals that yielded accurate electronic and optical properties for organic and inorganic molecules and semiconducting nanocrystals.

IMPACT By enabling computational characterization of defective states at a microscopic level, this project will provide knowledge and tools to interpret ongoing experiments on fuel production from water. This work will also help establish design rules for predicting robust qubits in wide-gap semiconductors.

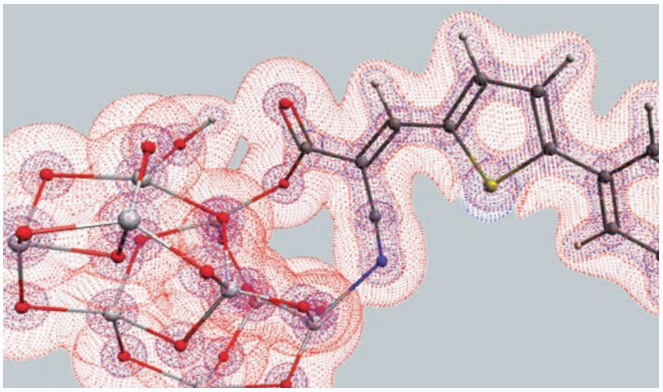
PUBLICATIONS

Brawand, Nicholas P., Marco Govoni, Marton Voros, and Giulia Galli. "Performance and Self-Consistency of the Generalized Dielectric Dependent Hybrid Functional," *Journal of Chemical Theory and Computation* (May 2017), ACS Publications.

Pham, T. A., M. Govoni, R. Seidel, S. E. Bradforth, E. Schwegler, and G. Galli. "Electronic Structure of Aqueous Solutions: Bridging the Gap between Theory and Experiments," *Science Advances* (June 2017), AAAS.

Data-Driven Molecular Engineering of Solar-Powered Windows

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



Isosurface of the Laplacian of the electron density of MK44, an organic dye, attached to the surface of a nanocluster of titania. *Image: Álvaro Vázquez Mayagoitia, Argonne National Laboratory; Jacqueline M. Cole, University of Cambridge*

CHALLENGE Dye-sensitized solar cells (DSC) are a strong contender for next-generation solar cell technology. Their transparent and low-cost nature makes them niche prospects for electricity-generating windows that will equip buildings for energy-sustainable future cities. Despite their vast industrial potential, DSC innovations are being held up by a lack of suitable light-harvesting dye chemicals.

APPROACH This work aims to discover new DSC dyes via a large-scale data mining approach. Prior to mining, suitable data must be sourced. Such data are being generated using a toolkit called ChemDataExtractor. This enables the automated extraction of chemical entities and their associated properties, measurements, and relationships from scientific documents that can be used to populate structured chemical databases. Natural language processing and machine learning are at the core of this tool. The chemistry literature is a good target for this automated extraction, as it is typically comprised of formulaic, data-rich language that is well suited for machine analysis with the potential for high recall and precision.

The data-mining process probes the databanks that have been constructed, with encoded forms of structure-property relationships, which explain the underlying physics and chemistry that govern good DSC dyes. These relationships are established using case studies on known DSC dyes, which are built up from a range of materials characterization efforts to support this dye discovery.

RESULTS Within this scope, case studies on dye molecules are being performed using calculations on Theta to complement the synchrotron-based experiments on known high-performance DSC dyes. This work has revealed new molecular design rules for DSC dyes that will help future materials prediction efforts. The team has also developed a new charge-transfer algorithm, which could provide a better way to encode certain descriptors for electronic structure calculations. They are verifying the algorithm via tests on case studies of experimentally determined molecular structures. Pending the final assessment of this evaluation process, this new algorithm development will represent a scientific contribution in its own right.

IMPACT Materials discovery of better-performing, light-absorbing dye molecules will be enabled via a synergistic computational and experimental science approach, wherein machine learning and data mining are used in conjunction with large-scale simulations and experiments to facilitate a materials-by-design workflow.

Petascale Simulations for Layered Materials Genome

PI Aiichiro Nakano
INST University of Southern California
HOURS INCITE, 140 Million Core-Hours

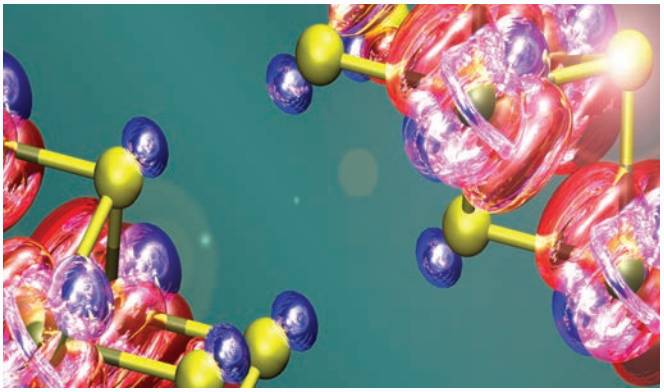


Photo-generated electron (red) and hole (blue) wave functions in bilayer $MoSe_2$, where gold and yellow spheres are molybdenum and selenium atoms, respectively. *Image: Lindsay Bassman, Aravind Krishnamoorthy, and Ken-ichi Nomura, University of Southern California*

CHALLENGE Functional layered materials are attractive for their outstanding electronic, optical, magnetic, and chemical properties, and for the tunable nature of these properties.

Layered materials can potentially contain unlimited combinations of atomically thin 2D layers, selected and stacked in optimal sequences for use in targeted applications, such as solar cells, batteries, and catalysis. This INCITE project is performing massive molecular dynamics simulations on ALCF supercomputers to validate experimental findings on layered materials, providing insights to advance the design and synthesis of such materials.

APPROACH The research team is carrying out nonadiabatic quantum molecular dynamics (NAQMD) and reactive molecular dynamics (RMD) simulations to aid in the synthesis of stacked, layered materials by chemical vapor deposition, exfoliation, and intercalation; and to discover function-property-structure relationships in the materials with a special focus on far-from-equilibrium electronic processes. Their simulations are being validated by experiments at SLAC National Accelerator Laboratory's Linac Coherent Light Source (LCLS) and Ultrafast Electron Diffraction (UED) facilities, providing predictive theory to support the DOE-funded MAterials Genome Innovation for Computational Software (MAGICS) Center at the University of Southern California. The simulation results will be integrated with MAGICS' computational linguistics and big data analytics efforts to advance efforts to build a layered materials genome.

RESULTS Photo-induced non-radiative energy dissipation is a potential pathway for inducing structural-phase transitions in layered 2D materials. To advance this field, a quantitative understanding of real-time atomic motion and lattice temperature is required. As part of a study published in *Nature Communications*, the INCITE team performed NAQMD simulations on Mira to corroborate the results of UED experiments on a bilayered semiconductor, molybdenum diselenide ($MoSe_2$). The simulations successfully reproduced the observed ultrafast increase in lattice temperature and the corresponding conversion of photoenergy to lattice vibrations. The results further suggest that a softening of vibrational modes in the excited state is involved in efficient and rapid energy transfer between the electronic system and the lattice.

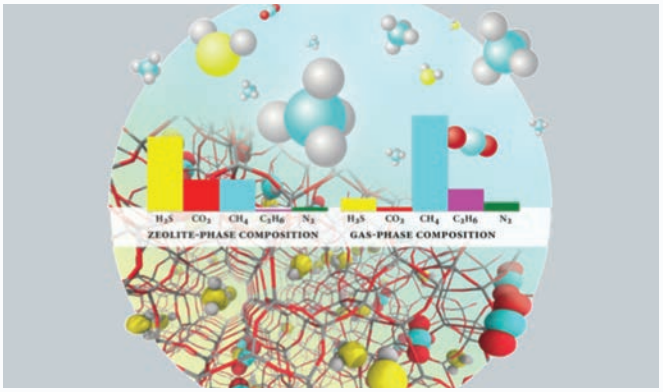
IMPACT By providing a better understanding of functional layered materials, this project is helping to accelerate the development of new materials for a wide range of energy, optoelectronic, and sensor applications. The team's simulation data will be widely disseminated to the scientific community through the Materials Project at Lawrence Berkeley National Laboratory.

PUBLICATIONS

Lin, Ming-Fu, Vidya Kochat, Aravind Krishnamoorthy, Lindsay Bassman, Clemens Weninger, Qiang Zheng, Xiang Zhang, Amey Apte, Chandra Sekhar Tiwary, Xiaozhe Shen, Renkai Li, Rajiv Kalia, Pulickel Ajayan, Aiichiro Nakano, Priya Vashishta, Fuyuki Shimojo, Xijie Wang, David M. Fritz, and Uwe Bergmann. "Ultrafast Non-radiative Dynamics of Atomically Thin $MoSe_2$," *Nature Communications* (November 2017), Springer Nature.

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

PI J. Ilja Siepmann
INST University of Minnesota
HOURS ALCC, 117 Million Core-Hours



Adsorption-based process for the removal of hydrogen sulfide and carbon dioxide from sour natural gas. *Image: Greg Chung, Pusan University; Evgenii O. Fetisov, Mansi Shap, and J. Ilja Siepmann, University of Minnesota*

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

APPROACH Scientists participating in the DOE-funded Nanoporous Materials Genome Center, led by the University of Minnesota, are using Mira to demonstrate and develop predictive theory and modeling tools that can rapidly screen thousands of materials to pinpoint promising candidates for further research. This project uses hierarchical screening workflows that involve machine learning, evolutionary algorithms, molecular simulations, and high-level electronic structure calculations.

Leveraging the MCCCS-MN, RASPA, and CP2K codes, the team's research is focused on performing (1) high-throughput screening to discover nanoporous materials with specific functions; (2) first-principles simulations of reactive phase and adsorption equilibria, and of electrolyte solutions in slit pores; and (3) electronic structure calculations to explore nanoporous materials and photovoltaic materials.

RESULTS In a paper published in *Nature*, the team used Mira to interpret experimental findings and predict the performance of zeolite-based separation membranes created using a newly developed synthesis method (patent pending). The groundbreaking fabrication process offers a more efficient and cost-effective method for producing zeolite nanosheets, which can be used to make ultra-selective, high-flux membranes. Calculations on Mira helped elucidate the nanosheet structure and transport barriers for xylene isomers, providing data that corroborated experimental measurements of ultra-high selectivities under operational conditions. In other studies, the team's simulations have led to the discovery of optimal zeolites for sweetening of highly sour natural gas streams and novel microporous materials for upgrading the research octane number of fuel mixtures.

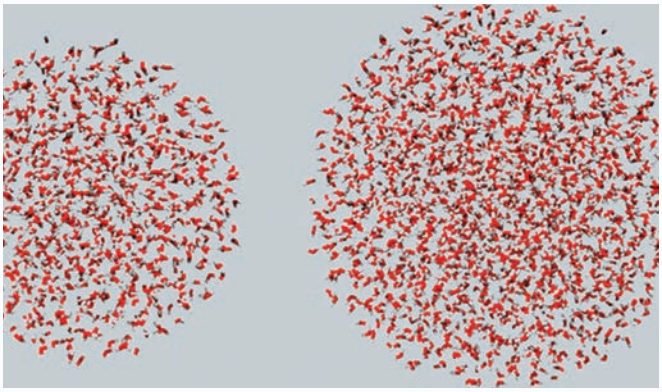
IMPACT With this project, researchers are developing improved predictive modeling capabilities to accelerate the discovery and design of nanoporous materials for complex chemical separation and transformation applications. The ability to identify optimal zeolites and metal-organic frameworks for specific energy applications has the potential to improve the production of biofuel and petroleum products, and advance the development of gas storage and carbon capture devices.

PUBLICATIONS

Jeon, Mi Young, Donghun Kim, Prashant Kumar, Pyung Soo Lee, Neel Rangnekar, Peng Bai, Meera Shete, Bahman Elyassi, Han Seung Lee, Katabathini Narasimharao, Sulaiman Nasir Basahel, Shaeel Al-Thabaiti, Wenqian Xu, Hong Je Cho, Evgenii O. Fetisov, Raghuram Thyagarajan, Robert F. DeJaco, Wei Fan, K. Andre Mkhoyan, J. Ilja Siepmann, and Michael Tsapatsis. "Ultra-Selective High-Flux Membranes from Directly Synthesized Zeolite Nanosheets," *Nature* (March 2017), Nature Publishing Group.

State-of-the-Art Simulations of Liquid Phenomena

PI Mark Gordon
INST Iowa State University
HOURS INCITE, 200 Million Core-Hours



Water clusters used for benchmarking on Mira. *Image: Yuri Alexeev, Graham Fletcher, and Spencer Pruitt, Argonne National Laboratory; Mark Gordon, Iowa State University; Kazuo Kitaura, Kobe University; Hiroya Nakata, Kyocera Corporation; Dmitri Fedorov and Takeshi Nagata, National Institute of Advanced Industrial Science and Technology (Japan); Maricris Mayes, University of Massachusetts Dartmouth*

CHALLENGE The process of a substance dissolving in a liquid—solvation—is critical to several energy-related applications, including solar cells, catalysts, and batteries. A better understanding of how solvated ions behave at or near an interface will aid in the design and optimization of various chemical reactions and processes used in the chemical and energy industries. Led by researchers from Iowa State University/Ames Laboratory and Argonne National Laboratory, this ALCF project is focused on the study of liquid behavior, both for a liquid itself and for the behavior of solutes in the liquid.

APPROACH To enable this research, the team used a fragment molecular orbital method within the GAMESS code to divide molecular systems into smaller units that can be solved quickly and simultaneously on Mira's highly parallel architecture. A key development has been the inclusion of three-body interactions at the level of second-order Møller-Plesset (MP2) perturbation thseory, which is needed to properly describe a cluster of water molecules.

The team performed simulations of water-solvated anions, in which the ion is represented by MP2 and the water is described by effective fragment potentials (EFP), and employed umbrella sampling to determine anion surface affinities more efficiently. Validating the MP2/EFP method for the study of anion surface affinity, they found it to be thousands of times cheaper than the full MP2 method. Previously scalable to only one rack of Mira, ALCF staff helped optimize and scale the new method in GAMESS to 16 racks.

RESULTS Using Mira, the team investigated properties of anions as they are solvated in water, specifically, the tendency of the anion to migrate to the surface of a water droplet. The study results, published in the *Journal of Chemical Theory and Computation*, highlight the importance of three-body terms in the relative energetics of water clusters. The requirement for methods to provide accurate three-body effects in water energetics emphasizes the need for three-body analytic gradients as a prerequisite for practical applications, such as water dynamics simulations.

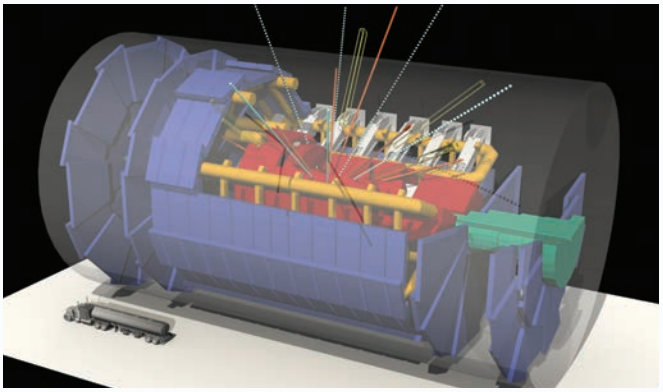
IMPACT This project is providing a methodical and accurate description and interpretation of the process of solvation for liquids that have increasing relevance in the development of energy-related applications.

PUBLICATIONS

Pruitt, Spencer R., Hiroya Nakata, Takeshi Nagata, Maricris Mayes, Yuri Alexeev, Graham Fletcher, Dmitri G. Fedorov, Kazuo Kitaura, and Mark S. Gordon. "Importance of Three-Body Interactions in Molecular Dynamics Simulations of Water Demonstrated with the Fragment Molecular Orbital Method," *Journal of Chemical Theory and Computation* 12, no. 4 (April 2016), ACS Publications.

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



Artist's representation of the ATLAS detector at CERN's Large Hadron Collider, showing particles produced in the aftermath of the collision between two high-energy protons (the truck shown in lower left is depicted for scale). *Image: Taylor Childers, Joseph A. Insley, and Thomas LeCompte, Argonne National Laboratory*

CHALLENGE Particle collision experiments at CERN's Large Hadron Collider (LHC) generate around 50 petabytes of data each year that must be processed and analyzed to aid in the facility's search for new physics discoveries. When CERN upgrades to the High Luminosity LHC in 2025, experimental data produced by the facility are expected to increase by a factor of 20. To help meet the LHC's growing computing needs, a research team is exploring the use of ALCF supercomputers to perform increasingly precise simulations, as well as calculations that are too intensive for traditional computing resources.

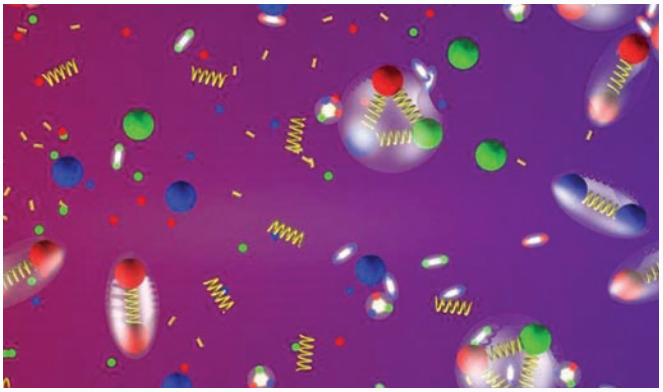
APPROACH This research builds on the progress of an ongoing ALCC project that is using Mira to perform event generation simulations for the LHC's ATLAS experiment. With the ADSP allocation, the research team is expanding its use of ALCF resources through the deployment of Athena, the ATLAS simulation and analysis framework, on Theta. Their ultimate goal is to develop an end-to-end workflow on ALCF computing resources that is capable of handling the ATLAS experiment's intensive computing tasks—event generation, detector simulations, reconstruction, and analysis.

RESULTS As a first step, the ALCF is working to deploy HTCondor-CE, a "gateway" software tool developed by the Open Science Grid to authorize remote users and provide a resource provisioning service. This effort requires writing code to allow HTCondor-CE to interact with the ALCF's job scheduler, Cobalt, as well as making modifications to the facility's authentication policy. To test this setup, the Argonne team has successfully carried out end-to-end production jobs on Cooley, paving the way for larger runs on Theta in the near future. With this tool in place, ATLAS researchers will be able to run jobs automatically through their workflow management system, simplifying the integration of ALCF resources as production compute endpoints for LHC experiments.

IMPACT The development of a workflow that integrates event generation and simulation on ALCF computing resources will increase the scientific reach of the ATLAS experiment. By enabling a portion of the LHC computing workload to run on ALCF supercomputers, researchers can speed the production of simulation results and accelerate efforts to search for evidence of new particles.

Fundamental Properties of QCD Matter Produced at RHIC and the LHC

PI Claudia Ratti
INST University of Houston
HOURS INCITE, 194 Million Core-Hours



The image illustrates how protons, neutrons, and other hadrons formed from quarks and gluons during the QCD transition as the universe expanded. Since the transition is a crossover, there is no sharp temperature, only a broad range where the transition happened. *Image: Sandor Katz, University of Budapest, Hungary*

CHALLENGE A few seconds after the Big Bang, the building blocks of matter emerged from a hot, energetic state known as the quark-gluon plasma (QGP). These building blocks of matter, called hadrons, form when gluons bind quarks together. Physicists are recreating the primordial conditions of the QGP in the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory, and the Large Hadron Collider (LHC) at CERN. Results suggest that the QGP is a strongly interacting system, which can be studied computationally through lattice quantum chromodynamics (QCD).

APPROACH Using experimental results and the JANOS QCD simulation code, researchers working on this continuing INCITE project are addressing the question of how the transition is modified if the pressure of the deconfined system is raised and the temperature is held constant. This is of particular interest since the collisions generated at RHIC at lower energies produce such a system, and it has been postulated that QCD matter will exhibit critical behavior near a critical point at finite density.

RESULTS Through expansion techniques, the team mapped out the phase diagram to densities characterized by chemical potentials that are twice the pseudo-critical temperature. No evidence for a critical point has been found, but the precision of the calculations enabled the development of effective theories based on equivalent gravitational equations used in black hole calculations. These theories now predict a critical point at chemical potentials as high as eight times the critical temperature.

Another key result is the calculation of observables, which verified the existence of a large number of additional hadronic states carrying strange quarks. These particles are needed to explain the experimental results of the transition behavior between the quark and hadronic phases. These short-lived states have to exist and they have to be populated during the transition. The calculations specify their mass, charge, quark composition, and decay properties, which will allow experimentalists to discover particles never seen before in nature.

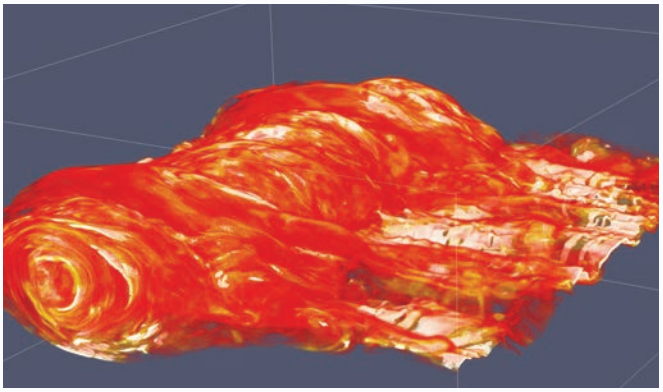
IMPACT The resulting data should help scientists determine the strength of coupling between quarks and gluons in the QGP, how charges propagate through it, and whether the QGP is the most ideal fluid ever observed.

PUBLICATIONS

Alba, Paolo, Rene Bellwied, Szabolcs Borsányi, Zoltan Fodor, Jana Günther, Sandor D. Katz, Valentina Mantovani Sarti, Jacquelyn Noronha-Hostler, Paolo Parotto, Attila Pasztor, Israel Portillo Vazquez, and Claudia Ratti. "Constraining the Hadronic Spectrum through QCD Thermodynamics on the Lattice," *Physical Review D* (August 2017), APS.

Kinetic Simulations of Relativistic Radiative Magnetic Reconnection

PI Dmitri Uzdensky
INST University of Colorado Boulder
HOURS INCITE, 90 Million Core-Hours



The electric current during relativistic magnetic reconnection in electron-positron plasma. *Image: Greg Werner, University of Colorado Boulder*

CHALLENGE Magnetic reconnection is a fundamental plasma physics process important in a great variety of both natural and laboratory plasma environments, from magnetic fusion devices to solar flares to intense high-energy X-ray and gamma-ray emissions from exotic astrophysical sources. Using very large kinetic numerical simulations, this project investigates high-energy particle acceleration and radiation caused by magnetic reconnection in the astrophysically relevant regime of relativistic, magnetically dominated plasma.

APPROACH To conduct its simulations, the team developed the radiative particle-in-cell code, Zeltron, which self-consistently incorporates the radiation reaction force on relativistic particles. The code was recently optimized to improve load balancing, greatly improving its performance on Mira.

RESULTS A comprehensive investigation of 3D magnetic reconnection in relativistic electron-positron pair plasmas demonstrated robust acceleration of particles into a nonthermal power law, despite potentially disruptive 3D instabilities. The nonthermal particle spectrum suggests that reconnection may explain observations of nonthermal spectra from distant astrophysical sources, such as the Crab Nebula's gamma-ray flares. A separate investigation of kinetic turbulence in relativistic electron-positron plasma has provided, for the first time using first-principles kinetic simulation, clear evidence that turbulent fluctuations can efficiently drive nonthermal particle acceleration to high energies, much like magnetic reconnection.

Both investigations show a similar dependence of the spectral power law index on the effective magnetization parameter, which characterizes the magnetic energy density relative to the relativistic inertia of the plasma. This similarity provides an important insight and benchmark for testing theoretical explanations of the underlying acceleration mechanisms. A comprehensive study of 2D electron-ion reconnection focused, for the first time, on the semi-relativistic regime of electron-ion reconnection. Results include the observation of electron acceleration to a nonthermal power law, the slope of which depends on magnetization parameters. Additionally, researchers found that reconnection decreases as magnetization parameters are lowered.

IMPACT Project results will lead to advances in the understanding of fundamental plasma physics processes and have important implications for modern high energy astrophysics. It will enable first-principles modeling of plasma energization and nonthermal particle acceleration in systems, such as pulsar wind nebulae and accretion flows, and jets powered by black holes.

PUBLICATIONS

Zhdankin, Vladimir, Gregory R. Werner, Dmitri A. Uzdensky, and Mitchell C. Begelman. "Kinetic Turbulence in Relativistic Plasma: From Thermal Bath to Nonthermal Continuum," *Physical Review Letters* (February 2017), APS.

ALCF Projects

2017 INCITE Projects

Biological Sciences

Biophysical Principles of Functional Synaptic Plasticity in the Neocortex

PI Eilif Muller
INST Blue Brain Project, EPFL
HOURS 100 Million Core-Hours

Chemistry

Towards Breakthroughs in Protein Structure Calculation and Design

PI David Baker
INST University of Washington
HOURS 150 Million Core-Hours

Understanding the Molecular Origin of Climate Change

PI Subramanian Sankaranarayanan
INST Argonne National Laboratory
HOURS 100 Million Core-Hours

Computer Science

Performance Evaluation and Analysis Consortium (PEAC) End Station

PI Leonid Oliker
INST Lawrence Berkeley National Laboratory
HOURS 60 Million Core-Hours
ALCF: 25M; OLCF: 35M

Earth Science

Frontiers in Planetary and Stellar Magnetism Through High-Performance Computing

PI Jonathan Aurnou
INST University of California, Los Angeles
HOURS 260 Million Core-Hours

Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations

PI Thomas Jordan
INST University of Southern California
HOURS 141 Million Core-Hours
ALCF: 45M; OLCF: 96M

High-Resolution Climate Change Simulations with the CESM

PI Gerald Meehl
INST National Center for Atmospheric Research
HOURS 215 Million Core-Hours

Accelerated Climate Modeling for Energy

PI Mark Taylor
INST Sandia National Laboratories
HOURS 278 Million Core-Hours
ALCF: 128M; OLCF: 150M

Engineering

Multiscale Physics of the Ablative Rayleigh-Taylor Instability

PI Hussein Aluie
INST University of Rochester
HOURS 47 Million Core-Hours

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

PI Kenneth E. Jansen
INST University of Colorado Boulder
HOURS 90 Million Core-Hours

LES to Characterize Shock Boundary Layer Interaction in a 3D Transonic Turbofan

PI Umesh Paliath
INST GE Global Research
HOURS 90 Million Core-Hours

Direct Numerical Simulation of Compressible, Turbulent Flow

PI Jonathan Poggie
INST Purdue University
HOURS 200 Million Core-Hours

Materials Science

Combining High Accuracy Electronic Structure Methods to Study Surface Reactions

PI Maria Chan
INST Argonne National Laboratory
HOURS 100 Million Core-Hours

Computational Spectroscopy of Heterogeneous Interfaces

PI Giulia Galli
INST The University of Chicago and Argonne National Laboratory
HOURS 200 Million Core-Hours

Electronic Stopping in Condensed Matter Under Ion Irradiation

PI Yosuke Kanai
INST University of North Carolina
HOURS 130 Million Core-Hours

Predictive Simulations of Functional Materials

PI Paul Kent
INST Oak Ridge National Laboratory
HOURS 138 Million Core-Hours
ALCF: 98M; OLCF: 40M

Materials and Interfaces for Organic and Hybrid Photovoltaics

PI Noa Marom
INST Carnegie Mellon University
HOURS 160 Million Core-Hours

Petascale Simulations for Layered Materials Genome

PI Aiichiro Nakano
INST University of Southern California
HOURS 140 Million Core-Hours

Reactive Mesoscale Simulations of Tribological Interfaces

PI Subramanian Sankaranarayanan
INST Argonne National Laboratory
HOURS 50 Million Core-Hours

Physics

The Rate of Spontaneous Plasma Reconnection

PI Andrey Beresnyak
INST U.S. Naval Research Laboratory
HOURS 52 Million Core-Hours

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 100 Million Core-Hours

Petascale Simulation of Magnetorotational Core-Collapse Supernovae

PI Sean Couch
INST Michigan State University
HOURS 100 Million Core-Hours

Cosmic Reionization on Computers

PI Nickolay Gnedin
INST Fermilab
HOURS 75 Million Core-Hours

Lattice QCD

PI Paul Mackenzie
INST Fermilab
HOURS 348 Million Core-Hours
ALCF: 240M; OLCF: 108M

Fundamental Properties of QCD Matter Produced at RHIC and the LHC

PI Claudia Ratti
INST University of Houston
HOURS 194 Million Core-Hours

Magnetohydrodynamic Models of Accretion Including Radiation Transport

PI James Stone
INST Princeton University
HOURS 54 Million Core-Hours

Petascale Simulations of Laser Plasma Interaction Relevant to IFE

PI Frank Tsung
INST University of California, Los Angeles
HOURS 147 Million Core-Hours

Nuclear Structure and Nuclear Reactions

PI James Vary
INST Iowa State University
HOURS 170 Million Core-Hours
ALCF: 80M; OLCF: 90M

PICSSAR—Particle-In-Cell Spectral Scalable Accurate Relativistic

PI Jean-Luc Vay
INST Lawrence Berkeley National Laboratory
HOURS 100 Million Core-Hours

2016–2017 ALCC Projects

Biological Sciences

Molecular Dynamics Studies of Biomass Degradation in Biofuel Production

PI Klaus Schulten
INST University of Illinois at Urbana-Champaign
HOURS 50 Million Core-Hours

Chemistry

Molecular Modeling of Hot Electron Transfer for Solar Energy Conversion

PI Hanning Chen
INST George Washington University
HOURS 16 Million Core-Hours

Computer Science

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications

PI Robert Voigt
INST Leidos
HOURS 191 Million Core-Hours
ALCF: 151M; OLCF: 40M

Earth Science

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

PI Peter Thornton
INST Oak Ridge National Laboratory
HOURS 211 Million Core-Hours
ALCF: 158M; OLCF: 53M

Engineering

Multiphase Simulations of Nuclear Reactor Flows

PI Igor Bolotnov
INST North Carolina State University
HOURS 72.1 Million Core-Hours

Computational Study of Cycle-to-Cycle Variation in Dual-Fuel Engines

PI Ravichandra Jupudi
INST GE Global Research
HOURS 25 Million Core-Hours

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

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

Adjoint-Based Optimization via Large-Eddy Simulation of a Fundamental Turbine Stator-Rotor

PI Qiqi Wang
INST Massachusetts Institute of Technology
HOURS 15 Million Core-Hours

Materials Science

First-Principles Design and Analysis of Energy-Efficient NanoElectronic Switches

PI Sefa Dag
INST GlobalFoundries
HOURS 10 Million Core-Hours

Computational Engineering of Defects in Soft and Hard Materials for Energy and Quantum Information Applications

PI Marco Govoni
INST The University of Chicago and Argonne National Laboratory
HOURS 53.7 Million Core-Hours

Modeling of Intense X-ray Laser Dynamics in Nanoclusters

PI Phay Ho
INST Argonne National Laboratory
HOURS 10 Million Core-Hours

The Materials Project—Completing the Space of Elastic and Piezoelectric Tensors

PI Kristin Persson
INST Lawrence Berkeley National Laboratory
HOURS 36 Million Core-Hours

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

PI J. Ilja Siepmann
INST University of Minnesota
HOURS 117 Million Core-Hours

First-Principles Design of Magnetic Materials, Models, and Mechanisms

PI Lucas Wagner
INST University of Illinois at Urbana-Champaign
HOURS 30 Million Core-Hours

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

PI Brian Wirth
INST University of Tennessee
HOURS 95 Million Core-Hours
ALCF: 70M; OLCF: 25M

Physics

High-Intensity Multibunch Physics in the Fermilab Accelerator Complex

PI James Amundson
INST Fermilab
HOURS 50 Million Core-Hours

Hadronic Light-by-Light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions

PI Thomas Blum
INST University of Connecticut
HOURS 180 Million Core-Hours

Extreme-Scale Gyrokinetic Particle Simulations to Complete the 2016 OFES National Theory/Simulation Performance Target and to Study the Fundamental Edge Physics

PI Choong-Seock Chang
INST Princeton Plasma Physics Laboratory
HOURS 175 Million Core-Hours
ALCF: 100M; OLCF: 75M

An End-Station for Intensity and Energy Frontier Experiments and Calculations

PI Taylor Childers
INST Argonne National Laboratory
HOURS 106.5 Million Core-Hours
ALCF: 93.5M; NERSC: 13M

***Ab Initio* Modeling of the Dynamical Stability of HED Plasmas: From Fusion to Astrophysics**

PI Frederico Fiuza
INST SLAC National Accelerator Laboratory
HOURS 60 Million Core-Hours

Exploring Higgs Compositeness Mechanism in the Era of the 14 TeV LHC

PI George Fleming
INST Yale University
HOURS 55 Million Core-Hours

Nuclear Structure for Tests of Fundamental Symmetries and Astroparticle Physics

PI Calvin Johnson
INST San Diego State University
HOURS 30 Million Core-Hours
ALCF: 6M; NERSC: 24M

Muon g-2 Hadronic Vacuum Polarization from Lattice QCD

PI John Laiho
INST Syracuse University
HOURS 66 Million Core-Hours

61-Pin Wire-Wrap Turbulent Conjugate-Heat Transfer: V&V for Industry and SESAME

PI Elia Merzari
INST Argonne National Laboratory
HOURS 120 Million Core-Hours

Numerical Simulation of Turbulent Flows in Advanced Steam Generators

PI Aleksandr Obabko
INST Argonne National Laboratory
HOURS 80 Million Core-Hours

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

PI Petros Tzeferacos
INST The University of Chicago
HOURS 60 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 and Argonne National Laboratory
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 156.8 Million Core-Hours
ALCF: 110M; OLCF: 46.8M

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

Engineering

Non-Boussines 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 and Argonne National Laboratory
HOURS 75 Million Core-Hours
ALCF: 60M; OLCF: 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 269.9 Million Core-Hours
ALCF: 80M; OLCF: 100M; NERSC: 89.9M

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

PI John T. 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

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

Nucleon Structure and Electric Dipole Moments with Physical Chirally Symmetric Quarks

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

2017 Director's Discretionary Projects

Biological Sciences

Exascale Deep Learning and Simulation Enabled Precision Medicine for Cancer

PI Rick Stevens
INST Argonne National Laboratory
HOURS 1 Million Core-Hours

Angora Scaling Study

PI Allen Taflove
INST Northwestern University
HOURS 9.9 Million Core-Hours

Chemistry

Ensemble Representation for the Realistic Modeling of Cluster Catalysts at Heterogeneous Interfaces

PI Anastassia N. Alexandrov
INST University of California, Los Angeles
HOURS 2.5 Million Core-Hours

Spectrum Slicing Eigensolver for *Ab Initio* Simulations

PI Murat Keceli
INST Argonne National Laboratory
HOURS 2 Million Core-Hours

Accurate Calculations of the Binding Energies of Dipole-Bound Anions

PI Brenda M. Rubenstein
INST Brown University
HOURS 7.5 Million Core-Hours

Comparison of Quantum Methods for Investigation of Protein-Ligand Binding Interactions

PI Vipin Sachdeva
INST IBM Research
HOURS 1 Million Core-Hours

Fragment Molecular Orbital (FMO) and Effective Fragment Molecular Orbital (EFMO) Methods for Exascale Computing

PI Federico Zaharie
INST Iowa State University, Ames
HOURS 6 Million Core-Hours

Computer Science

SciDAC Scalable Data Management Analysis and Visualization

PI Michael E. Papka, Joseph A. Insley
INST Argonne National Laboratory
HOURS 1 Million Core-Hours

MPICH—A High Performance and Widely Portable MPI Implementation

PI Ken Raffenetti
INST Argonne National Laboratory
HOURS 26 Million Core-Hours

Interfacial Behavior of Alcohol at Water/Organic Biphasic System

PI Baofu Qiao
INST Argonne National Laboratory
HOURS 5 Million Core-Hours

Portable Application Development for Next-Generation Supercomputer Architectures

PI Tjerk Straatsma, Katerina B. Antypas, Timothy J. Williams
INST Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory, and Argonne National Laboratory
HOURS 5 Million Core-Hours

ExaHDF5: Advancing HDF5 HPC I/O to Enable Scientific Discovery

PI Venkat Vishwanath
INST Argonne National Laboratory
HOURS 2 Million Core-Hours

Extreme Many-Task Computing with Swift

PI Justin M. Wozniak
INST Argonne National Laboratory
HOURS 1.2 Million Core-Hours

Earth Science

Simulating Global Terrestrial Carbon Sequestration and Carbon Transport to Aquatic Ecosystems—Pilot Study

PI Jinxun Liu
INST U.S. Geological Survey
HOURS 2 Million Core-Hours

Energy Technologies

TAE Technologies FRC Whole Device Modeling—Phase 1

PI Sean Dettrick
INST TAE Technologies
HOURS 5 Million Core-Hours

Modeling and Prediction of Nanocatalysts for Fuel Cells

PI Binay Prasai
INST Central Michigan University
HOURS 2 Million Core-Hours

NEAMS Neutronics Verification and Validation Simulations

PI Emily Shemon
INST Argonne National Laboratory
HOURS 7 Million Core-Hours

Domain Decomposed 3D Method of Characteristics Reactor Simulation Study

PI John Tramm
INST Massachusetts Institute of Technology
HOURS 1 Million Core-Hours

Advancing Understanding of Fission Gas Behavior in Nuclear Fuel Through Leadership-Class Computing

PI Brian Wirth
INST The University of Tennessee, Knoxville
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Engineering

Multiphase Simulations of Nuclear Reactor Thermal Hydraulics

PI Igor A. Bolotnov
INST North Carolina State University
HOURS 5 Million Core-Hours

Variable-Density Fluid Dynamics

PI Paul E. Dimotakis
INST California Institute of Technology
HOURS 10 Million Core-Hours

Numerical Simulation of Acoustic Radiation from High-Speed Turbulent Boundary Layers

PI Lian Duan
INST Missouri University of Science and Technology
HOURS 3 Million Core-Hours

Variable-Density Turbulence under Variable Acceleration

PI Daniel Livescu
INST Los Alamos National Laboratory
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Simulation of Supersonic Combustion

PI Farzad Mashayek
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Data Analysis of Turbulent Channel Flow at High Reynolds Number

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Influence on Duct Corner Geometry on Secondary Flow: Convergence from Duct to Pipe Flow

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

PI Joseph W. Nichols
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Investigation of a Low-Octane Gasoline Fuel for a Heavy-Duty Diesel Engine in a Low-Temperature Combustion Regime

PI Sibendu Som
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Materials Science

Large-Scale *Ab Initio* Simulations of Crystal Defects

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Physics

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2016–2017 ADSP Projects

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

PI Taylor Childers
INST Argonne National Laboratory

Data-Driven Molecular Engineering of Solar-Powered Windows

PI Jacqueline M. Cole
INST University of Cambridge

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

PI Fabien Delalondre
INST Blue Brain Project, EPFL

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

PI Doga Gursoy
INST Argonne National Laboratory

2017–2018 ADSP Projects

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

Realistic Simulations of the LSST Survey at Scale

PI Katrin Heitmann
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Constructing and Navigating Polymorphic Landscapes of Molecular Crystals

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Theta ESP Projects

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

PI Volker Blum
INST Duke University

Large-Scale Simulation of Brain Tissue

PI Fabien Delalondre
INST Blue Brain Project, EPFL

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

PI Christos Frouzakis
INST ETH Zürich

First-Principles Simulations of Functional Materials for Energy Conversion

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Quantum Monte Carlo Calculations in Nuclear Theory

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Free Energy Landscapes of Membrane Transport Proteins

PI Benoît Roux
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Aurora ESP Projects

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High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang
INST Princeton Plasma Physics Laboratory

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

PI Thomas Dunning
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Extreme-Scale Simulations for Multi-Wavelength Cosmology Investigations

PI Katrin Heitmann
INST Argonne National Laboratory

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INST University of Colorado Boulder

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Free Energy Landscapes of Membrane Transport Proteins

PI Benoît Roux
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January

The ATLAS Collaboration. "Measurement of the ZZ Production Cross Section in Proton–Proton Collisions at $\sqrt{s}$=8 TeV Using the ZZ → $\ell^-\ell^+\ell'^-\ell'^+$ and ZZ→$\ell^-\ell^+\nu\nu^-$ Decay Channels with the ATLAS Detector," *Journal of High Energy Physics* (January 2017), Springer Berlin Heidelberg. doi:10.1007/JHEP01(2017)099.

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February

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March

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Editorial Team: Beth Cerny (Project Lead), Jim Collins (Lead Writer), Karen Fellner, Mary Fitzpatrick, Andrea Manning, John Spizzirri, and Laura Wolf

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CONTACT
media@alcf.anl.gov
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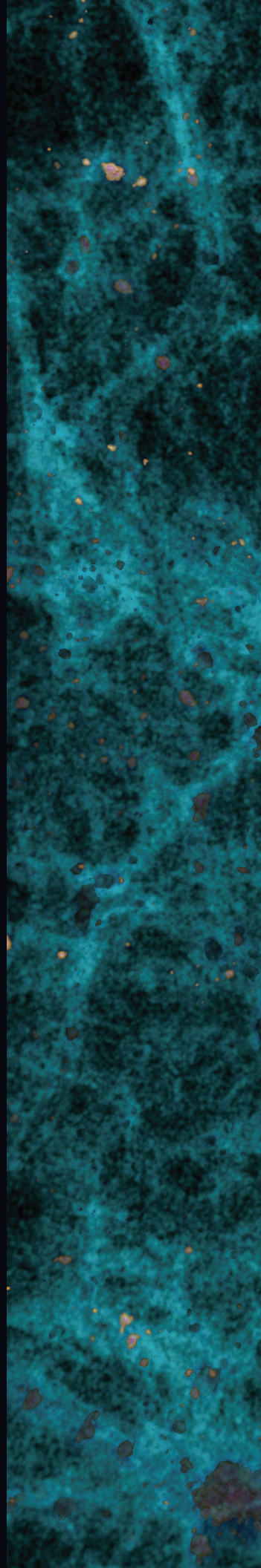

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