Argonne Leadership Computing Facility

2018 Annual Report

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

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2018 Annual Report

YEAR IN REVIEW

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

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

ALCF Leadership

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

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

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

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

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

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

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

MICHAEL E. PAPKA
ALCF Director

JINI RAMPRAKASH
ALCF Deputy Director

MARK FAHEY
ALCF Director of Operations

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

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

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

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

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

In 2018, we made several enhancements to the ALCF computing environment. Our staff deployed a Continuous Integration (CI) solution using an open-source Jenkins automation server, providing users with a tool that can accelerate efforts to build, test, and optimize their codes for ALCF systems. We are working with DOE's Exascale Computing Project to set up a separate solution based on GitLab with the intention of providing seamless CI abilities across DOE laboratories. We significantly upgraded our tape archive infrastructure with the deployment of LTO8 tape technology, which offers five times the capacity (12 TB) and more than double the transfer rate (360 MB/s) of our previous tape drives. In the business intelligence space, we launched new web-based reporting capabilities that provide up-to-date system data and metrics for both users and staff members.

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

KATHERINE RILEY
ALCF Director of Science

KALYAN KUMARAN
ALCF Director of Technology

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

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

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

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

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

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

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

ALCF at a Glance

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

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

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

Core-hours of compute time

8.7B

Active projects*

410

Facility users*

954

Publications

276

Supercomputers on the Top500 list

3

Fiscal year 2018

2018 ALCF Users by Affilliation
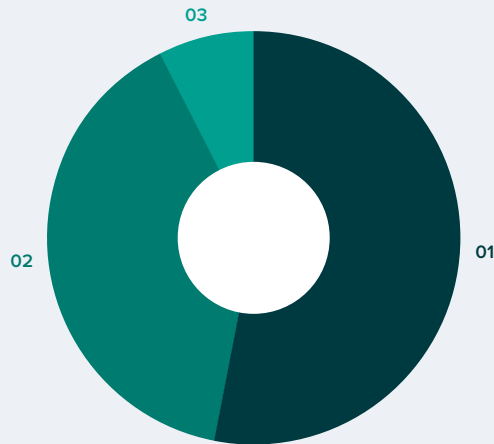
01 Academia

507

02 Government

376

03 Industry

71

2018 U.S. ALCF Users by State
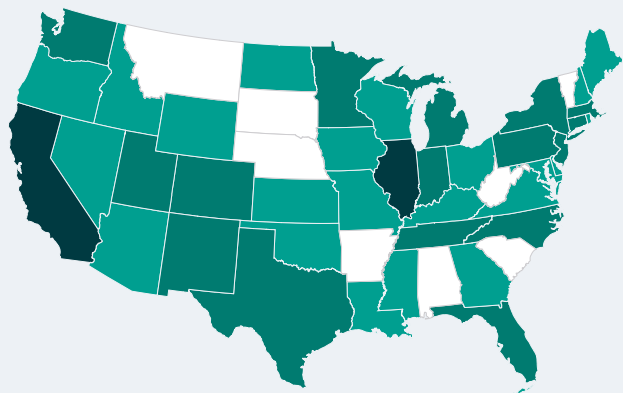
100+ Users

California   Illinois

11–100 Users

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

01–10 Users

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

PREPARING FOR EXASCALE

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

The ALCF's Exascale Future

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

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

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

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

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

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

While simulation has long been the cornerstone of scientific computing, the ALCF has been working to create an environment that also supports data science and machine learning-based research for the past few years.

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

In addition, Argonne recently created the Computational Science Division and the Data Science and Learning Division to explore challenging scientific problems through advanced modeling and simulation, and data analysis and artificial intelligence methods, respectively.

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

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

Aurora, the ALCF's future exascale system, will
help ensure continued U.S. leadership in high-end
computing for scientific research.
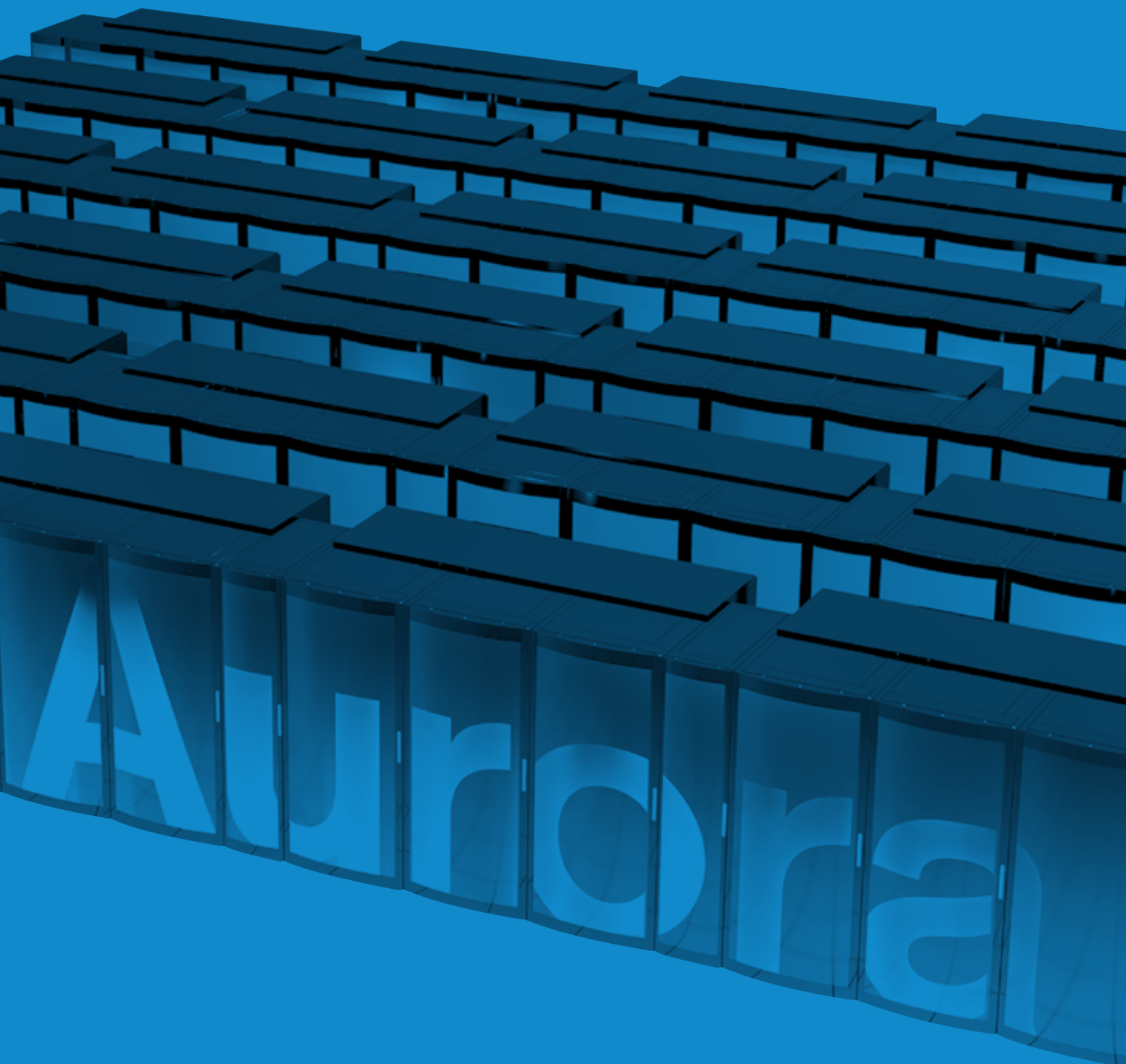
Secretary of Energy Rick Perry (second from right) toured the Argonne Leadership Computing Facility with Rick Stevens, Associate Laboratory Director for Argonne's Computing, Environment and Life Sciences Directorate (third from left). Accompanying the Secretary were Argonne Director Paul Kearns, U.S. Representative Bill Foster, DOE's Joanna Livengood, and others.

ADVANCING SCIENCE WITH DATA-CENTRIC TOOLS AND SERVICES

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

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

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

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

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

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

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

TRAINING USERS ON EMERGING HPC TOOLS AND TECHNIQUES

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

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

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

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

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

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

ARGONNE TESTBEDS ENABLE PIONEERING COMPUTING RESEARCH

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

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

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

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

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

PARTNERING WITH DOE'S EXASCALE COMPUTING PROJECT

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

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

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

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

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

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

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

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

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

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

Readying Aurora for Science on Day One

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

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

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

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

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

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

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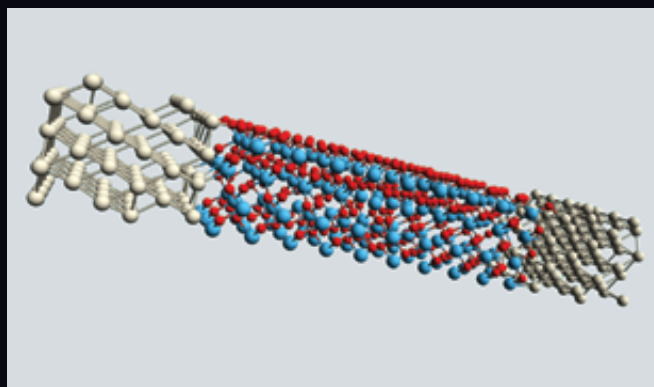
Hafnium oxide semiconductor with oxygen vacancies representing the oxygen leakage, inserted between platinum contacts at both ends. *Image: Olle Heinonen, Argonne National Laboratory*

SIMULATION

Extending Moore's Law Computing with Quantum Monte Carlo

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

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

DEVELOPMENT
The development of QMCPACK focuses on enabling the code's kernel to run efficiently on the exascale system, while managing multi-level memory/storage hierarchy and exposing additional layers of parallelism. The team also worked on improving high-throughput internal tools to drive large campaign runs on Aurora.
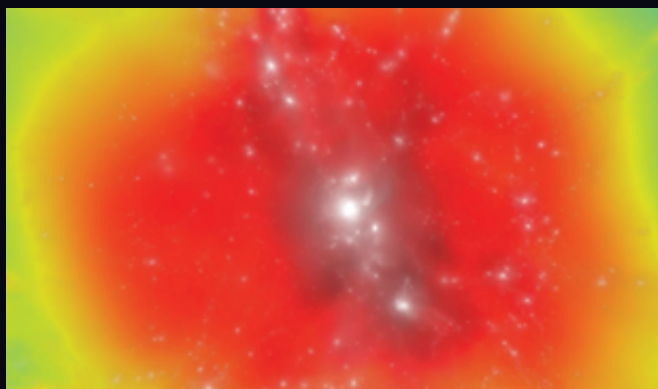
This image shows the baryon density (white) and the baryon temperature (color) of a cluster of galaxies. *Image: JD Emberson and the HACC team, Argonne National Laboratory*

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

Extreme-Scale Cosmological Hydrodynamics

PI	Katrin Heitmann
INST	Argonne National Laboratory
SFTWR	HACC, Thrust

SCIENCE

Researchers will use Aurora to perform cosmological hydrodynamics simulations that cover the enormous length scales characteristic of large sky surveys, while at the same time capturing the relevant small-scale physics. These simulations will help guide and interpret observations from large-scale cosmological surveys.

DEVELOPMENT

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

Extreme-Scale Unstructured Adaptive CFD

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

SCIENCE

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

DEVELOPMENT

The strong scaling needs of PHASTA will help stress test and improve Aurora's advanced interconnect. PHASTA's I/O capabilities will be enhanced to take advantage of Aurora's I/O system. This project will also make use of PETSc, PUMI, and Zoltan, preparing these libraries for future use on Aurora.
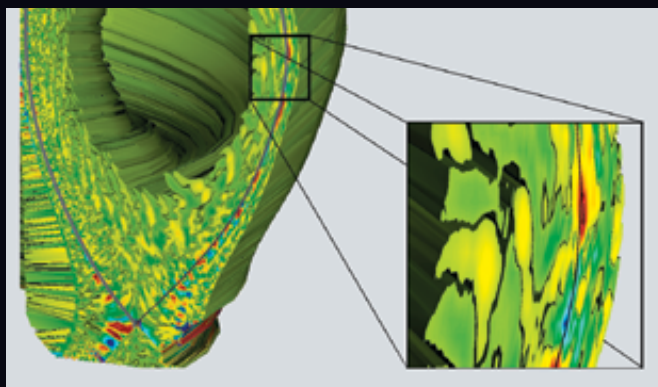
Structure of density eddies from plasma turbulence in a typical present-day tokamak edge plasma. The transition from a connected core-like turbulence eddies to isolated turbulence across the magnetic separatrix surface (black line) can be seen. *Image: Dave Pugmire, Oak Ridge National Laboratory; Seung-Hoe Ku, Princeton Plasma Physics Laboratory*

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

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

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

SCIENCE

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

DEVELOPMENT

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

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

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

SCIENCE

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

DEVELOPMENT

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

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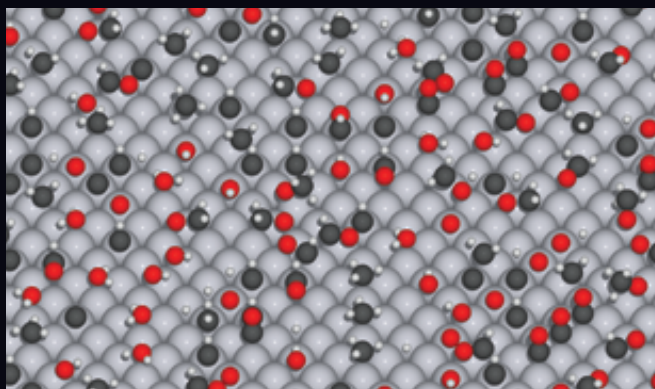
Data science techniques will be used in combination with quantum chemistry simulations to explore the otherwise intractable phase space resulting from gas phase molecules on catalyst surfaces to find relevant configurations and the lowest transition states between them. *Image: Eric Hermes, Sandia National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

DATA

Exascale Computational Catalysis

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

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

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

DATA/LEARNING METHODS
Regression, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, image and signal processing, databases, and graph analytics
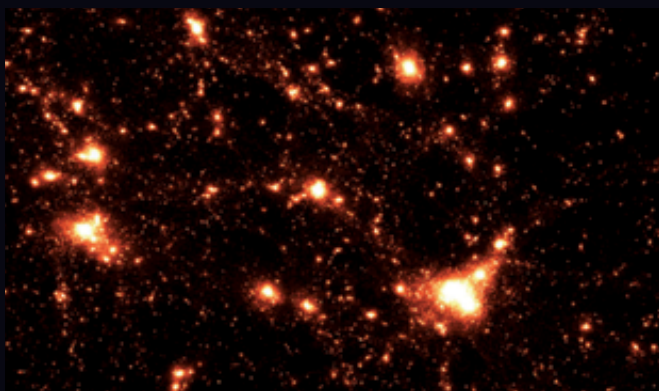
HACC cosmology simulations allow researchers to track the evolution of structures in great detail. *Image: Joseph A. Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory*
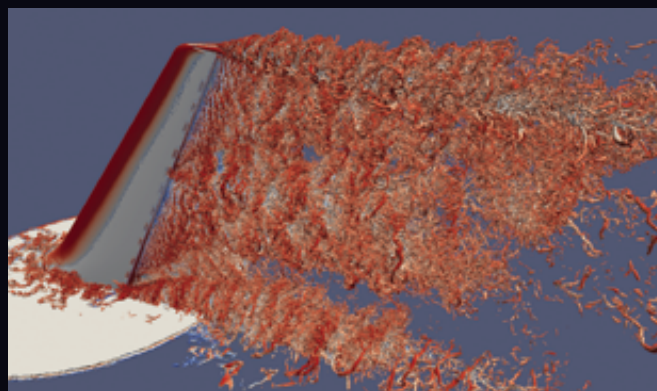
Flow visualization through an isosurface of instantaneous Q criterion colored by speed. *Image: Kenneth Jansen, University of Colorado Boulder*

Dark Sky Mining

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

SCIENCE

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

DEVELOPMENT

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

DATA/LEARNING METHODS

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

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

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

SCIENCE

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

DEVELOPMENT

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

DATA/LEARNING METHODS

Regression, uncertainty quantification, advanced workflows, advanced statistics, reduced/surrogate models, in situ visualization and analysis, and image and signal processing
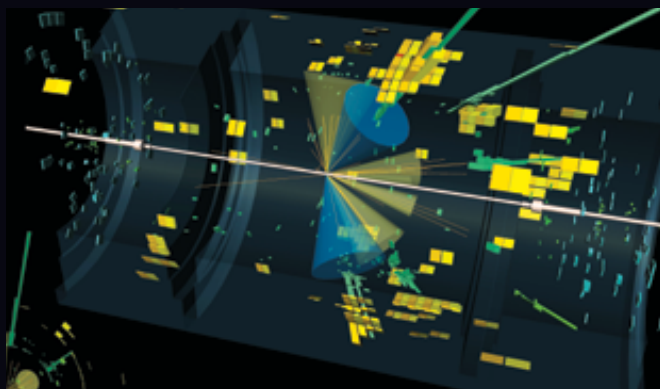
A candidate event in which a Higgs boson is produced in conjunction with top and anti-top quarks which decay to jets of particles. The challenge is to identify and reconstruct this type of event in the presence of background processes with similar signatures which are thousands of times more likely. *Image: CERN*
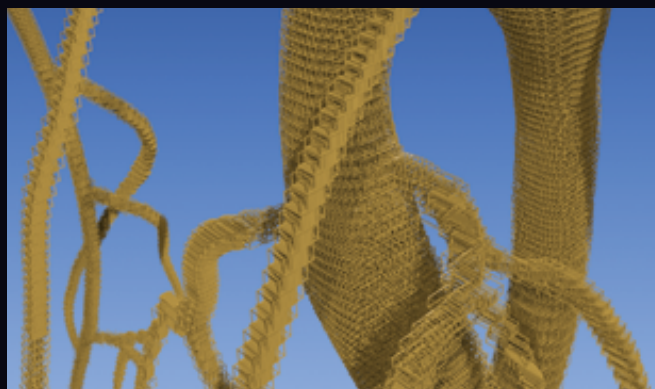
Capturing flow in the human aorta requires high-resolution fluid models. In this case, the wireframe boxes indicate each computational bounding box describing the work assigned to an individual task. *Image: Liam Krauss, Lawrence Livermore National Laboratory*

Simulating and Learning in the ATLAS Detector at the Exascale

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

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

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

DATA/LEARNING METHODS
Classification, clustering, dimensionality reduction, advanced workflows, advanced statistics, image and signal processing, and databases

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

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

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

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

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

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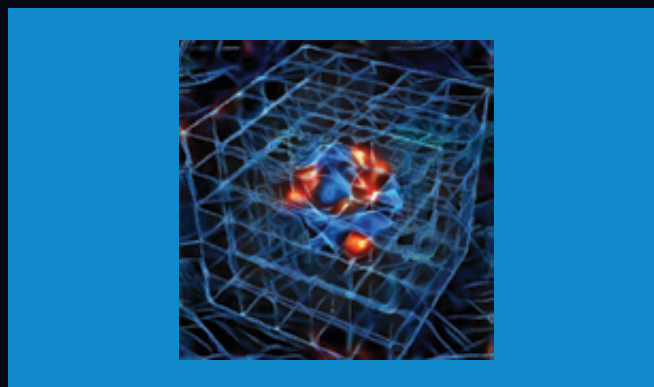
Researchers will couple machine learning and lattice QCD simulations to advance the study of nuclei. This artistic rendering was created with deepart.io.
Image: William Detmold and Phiala Shanahan, Massachusetts Institute of Technology

LEARNING

Machine Learning for Lattice Quantum Chromodynamics

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

SCIENCE

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

DEVELOPMENT

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

DATA/LEARNING METHODS

Classification, regression, reinforcement learning, clustering, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, and databases
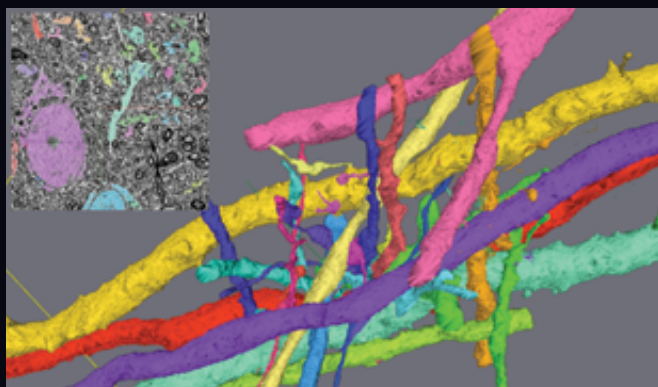
Neurons rendered from the analysis of electron microscopy data. The inset shows a slice of data with colored regions indicating identified cells. Tracing these regions through multiple slices extracts the sub-volumes corresponding to anatomical structures of interest. *Image: Nicola Ferrier, Narayanan (Bobby) Kasthuri, and Rafael Vescovi, Argonne National Laboratory*

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

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

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

SCIENCE
This project will develop a computational pipeline for neuroscience that will extract brain-image-derived mappings of neurons and their connections from electron microscope datasets too large for today's most powerful systems.

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

DATA/LEARNING METHODS
Classification, regression, clustering, uncertainty quantification, advanced workflows, advanced statistics, image and signal processing, and graph analytics

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

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

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

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

DATA/LEARNING METHODS
Classification, regression, clustering, uncertainty quantification, dimensionality reduction, advanced workflows, advanced statistics, reduced/surrogate models, and databases
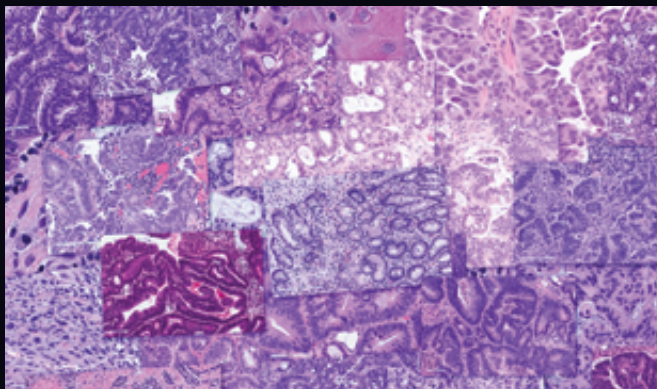
Predicting cancer type and drug response using histopathology images from the National Cancer Institute's Patient-Derived Models Repository. *Image: Rick Stevens, Argonne National Laboratory*

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

Virtual Drug Response Prediction

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

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

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

DATA/LEARNING METHODS
Classification, regression, clustering, uncertainty quantification, dimensionality reduction, advanced workflows, and image and signal processing

Accelerated Deep Learning Discovery in Fusion Energy Science

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

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

DEVELOPMENT
The FRNN software stack will stress the system's deep learning capabilities and software stack. Large data-parallel training and hyperparameter optimization requirements will stress Aurora's communication fabric and stand to benefit from the system's I/O hardware.
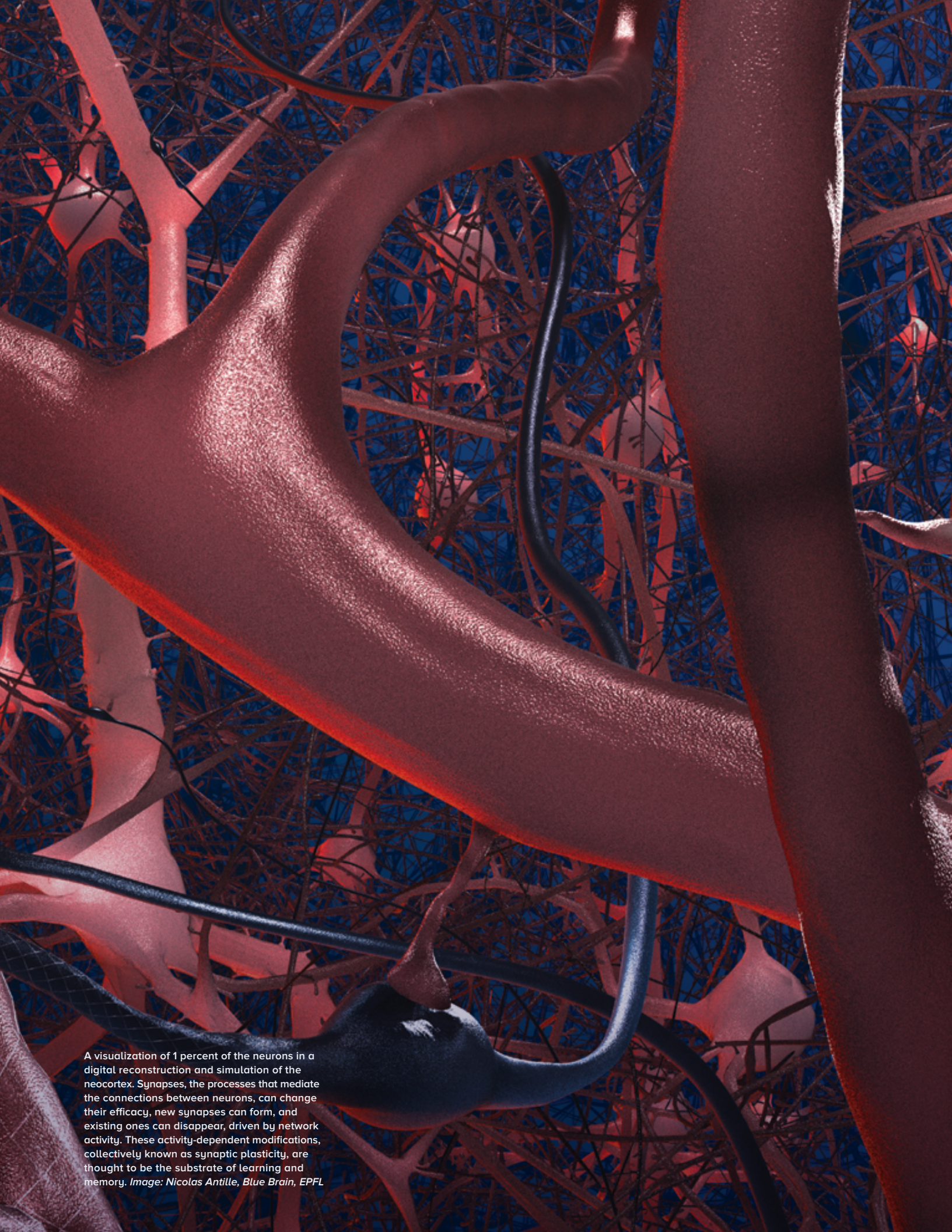
DATA/LEARNING METHODS
Classification, regression, clustering, and dimensionality reduction

GROWING THE HPC COMMUNITY

As a leader in the HPC community, the ALCF is actively involved in efforts to broaden the impact of supercomputers and grow the body of researchers who can use them to advance science.
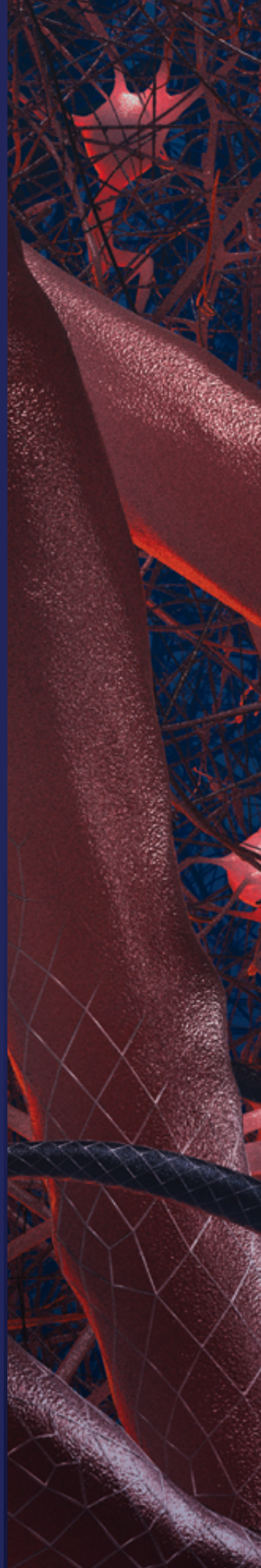
A visualization of 1 percent of the neurons in a digital reconstruction and simulation of the neocortex. Synapses, the processes that mediate the connections between neurons, can change their efficacy, new synapses can form, and existing ones can disappear, driven by network activity. These activity-dependent modifications, collectively known as synaptic plasticity, are thought to be the substrate of learning and memory. *Image: Nicolas Antille, Blue Brain, EPFL*

Partnering with Industry to Enable High-Impact Research

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

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

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

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

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

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

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

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

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

Kinetic Simulation of Field-Reversed Configuration Stability and Transport

PI   Sean Dettrick
INST   TAE Technologies

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

Advancing Computer-Aided Drug Design

PI   Vipin Sachdeva
INST   Silicon Therapeutics

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

Enabling Multiscale Physics for Industrial Design Using Deep Learning Networks

PI   Rathakrishnan Bhaskaran
INST   GE Global Research

GE Global Research's ALCF Data Science Program project is focused on leveraging machine learning and large datasets generated by wall-resolved large-eddy simulations to develop data-driven turbulence models with improved predictive accuracy. The researchers will apply this approach to turbomachinery, such as a wind turbine airfoil, demonstrating the impact that deep learning can have on industrial design processes for applications in power generation, aerospace, and other fields.
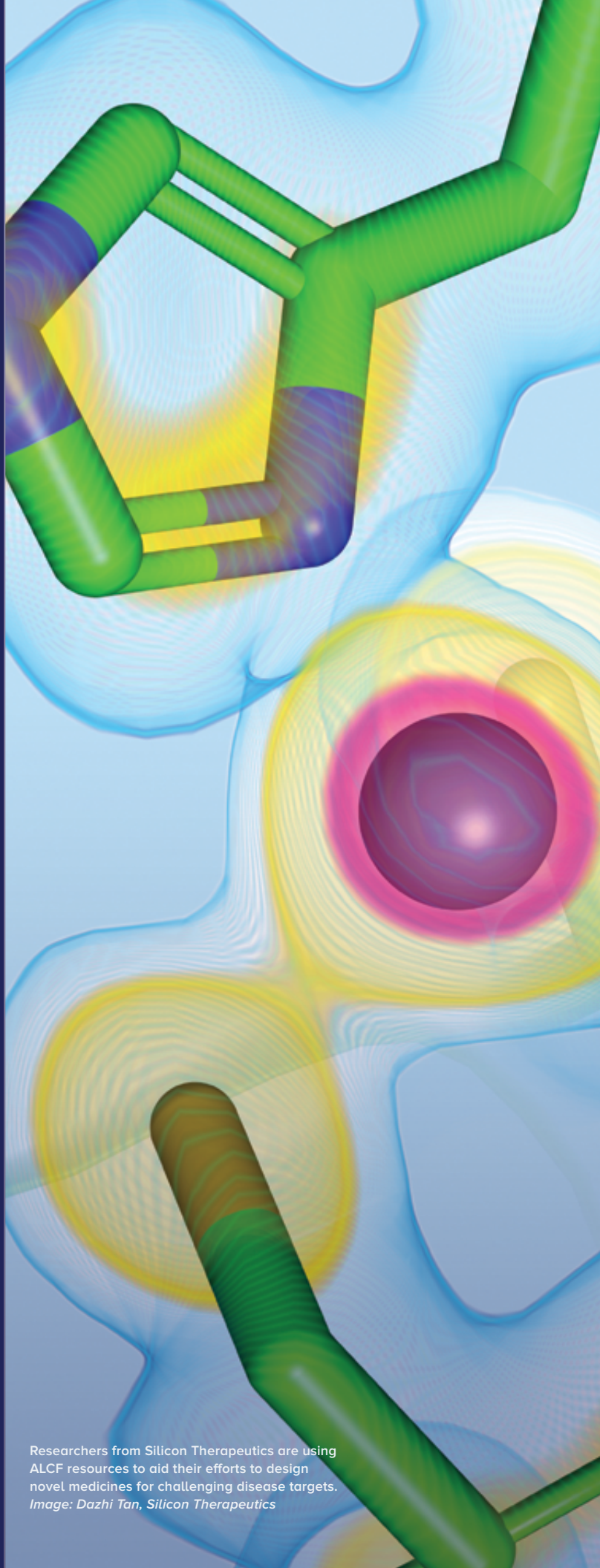
Researchers from Silicon Therapeutics are using ALCF resources to aid their efforts to design novel medicines for challenging disease targets.
Image: Dazhi Tan, Silicon Therapeutics

Shaping the Future of Supercomputing

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

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

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

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

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

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

Community Activities

Computational Neuroscience Workshop

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

Exascale Computing Project

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

HPC Standards, Benchmarks, and Technologies

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

Intel eXtreme Performance Users Group

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

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

Lustre Users Group Conference

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

Performance Portability

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

Quantum Computing Training

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

SC18

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

Engaging Current and Future HPC Users

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

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

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

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

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

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

Inspiring Students

Big Data and Visualization Camp

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

CodeGirls@Argonne Camp

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

Hour of Code

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

National Science Bowl

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

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

SC18 Student Cluster Competition

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

Summer Coding Camp

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

Summer Student Program

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

Women in STEM

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

Training Users

ALCF Computational Performance Workshop

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

ALCF Getting Started Videoconferences

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

ATPESC 2018

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

Aurora Early Science Program Training Series

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

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

Best Practices for HPC Software Developers

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

Many-Core Developer Sessions

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

Simulation, Data, and Learning Workshops

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

EXPERTISE AND RESOURCES

The ALCF's unique combination of supercomputing resources and expertise enables breakthroughs in science and engineering that would otherwise be impossible.
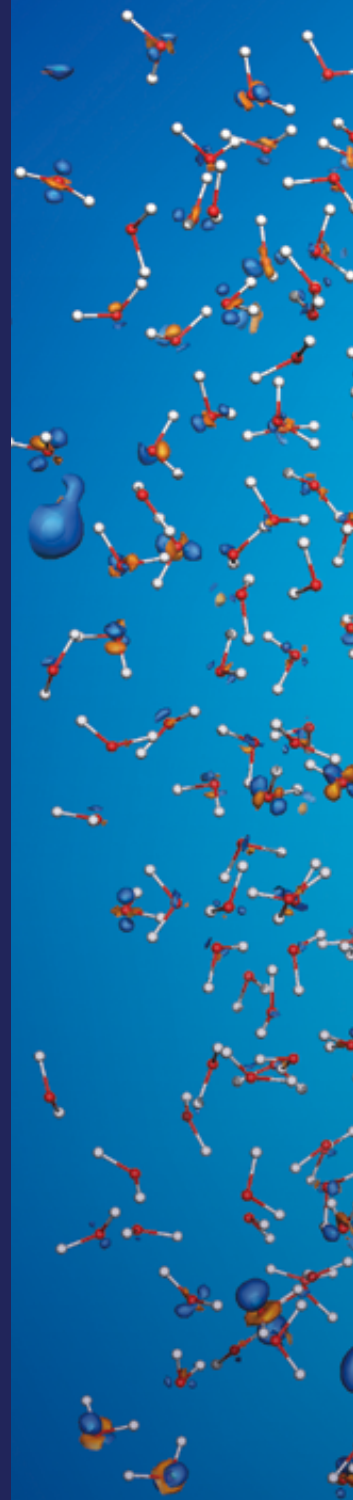
A snapshot from a non-equilibrium electron dynamics simulation of DNA in water under proton irradiation. The blue and orange isosurface represents areas with positive and negative changes in electron density with respect to the equilibrium density.
Image: Dillon C. Yost, University of North Carolina at Chapel Hill

The ALCF Team

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

OPERATIONS

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

SCIENCE AND TECHNOLOGY

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

OUTREACH

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

Staff News

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

KUMARAN RECEIVES 2018 SPEC PRESIDENTIAL AWARD

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

HARMS WINS R&D 100 AWARD

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

MESSINA SELECTED FOR DISTINGUISHED SERVICE AWARD

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

BRIGGS RECEIVES SCSW FOUNDERS AWARD

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

Staff Spotlights

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

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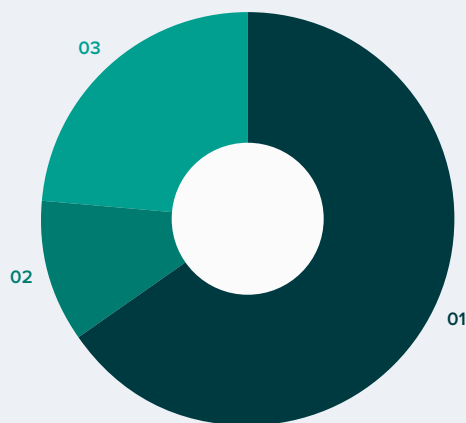
01 Staff Members

95

02 Postdoctoral Researchers

16

03 Summer Students

34

THOMAS APPLENCOURT
Computational Scientist

COLLEEN BERTONI
Computational Scientist

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

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

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

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

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

TAYLOR CHILDERS
Computer Scientist

GORDON MCPHEETERS
HPC Systems Administrator—File Systems

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

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

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

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

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

JEFF NEEL
Cyber Security Engineer/HPC Systems Administrator

HARITHA SIDDABATHUNI SOM
User Experience Team Lead

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

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

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

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

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

ALCF Computing Resources

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

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

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

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

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

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

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

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

ALCF Computing Systems

Mira

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

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

Theta

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

Intel-Cray XC40 architecture	4,392 nodes	70 TB of high-bandwidth memory
11.69 petaflops	281,088 cores	
64-core, 1.3-GHz Intel Xeon Phi 7230 processor per node	843 TB of 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	16-core, 1.6-GHz IBM PowerPC A2 processor per node	64 TB of memory
838 teraflops	4,096 nodes	5D torus interconnect
	65,536 cores	4 racks

Iota

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

Intel-Cray XC40 architecture	44 nodes	1 TB of high-bandwidth memory
117 teraflops	2,816 cores	
64-core, 1.3-GHz Intel Xeon Phi 7230 processor per node	12.3 TB of 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	16-core, 1.6-GHz IBM PowerPC A2 processor per node	32 TB of memory
419 teraflops	2,048 nodes	5D torus interconnect
	32,768 cores	2 racks

Cooley

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

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

Supporting Resources

Data Storage

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

DISK STORAGE

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

TAPE STORAGE

The ALCF has three 10,000-slot libraries. The tape technology is currently undergoing an upgrade to replace LTO-6 tape drives with LTO-8 tape drives. The upgrade should ultimately provide up to 300 PB of effective storage (approximately five times the amount provided by the LTO-6 tapes).

Networking

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

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

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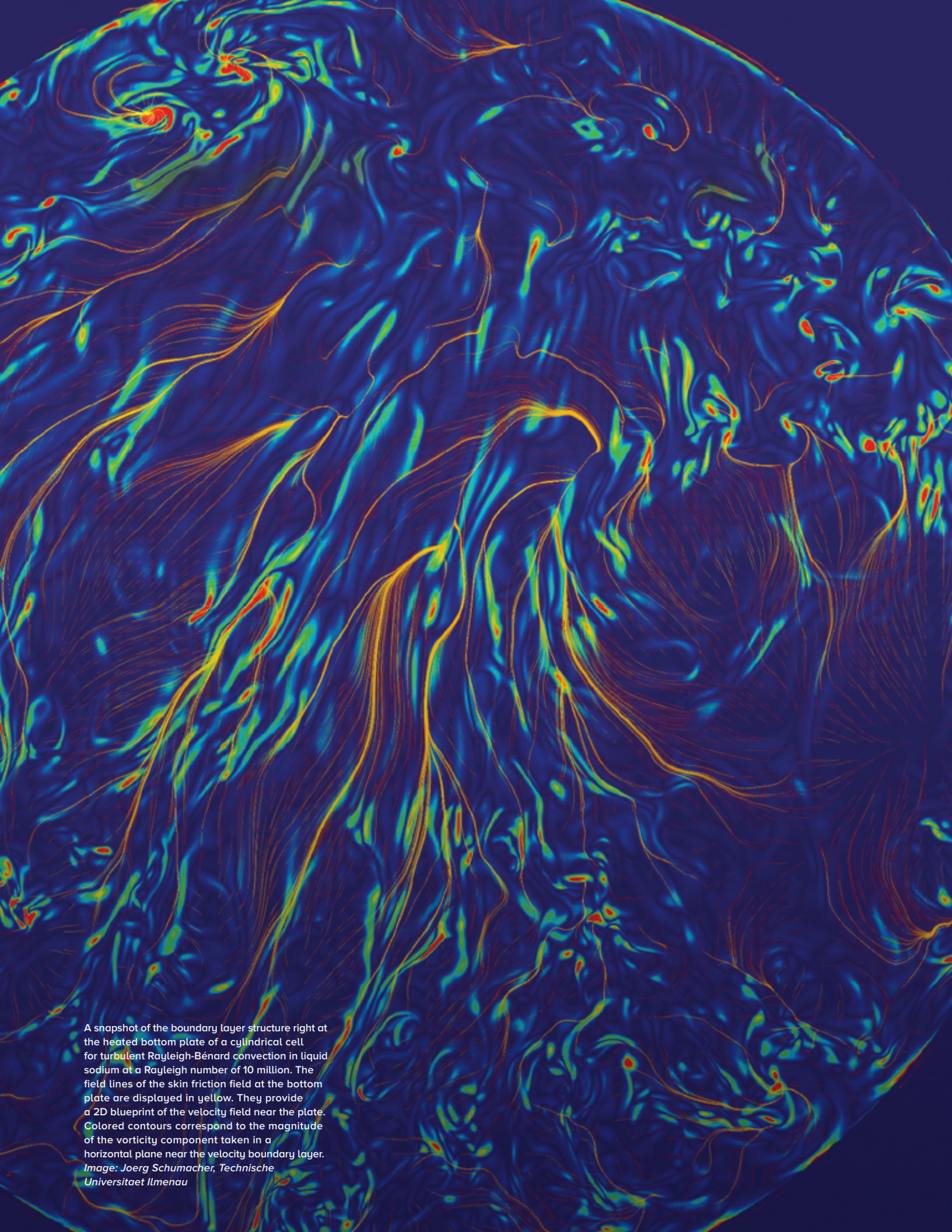
Through Argonne's Joint Laboratory for System Evaluation, the ALCF provides access to next-generation hardware and software to explore low-level experimental computer and computational science, including operating systems, messaging, compilers, benchmarking, power measurements, I/O, and new file systems.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

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

The ALCF is accelerating scientific discoveries in many disciplines, ranging from chemistry and engineering to physics and materials science.
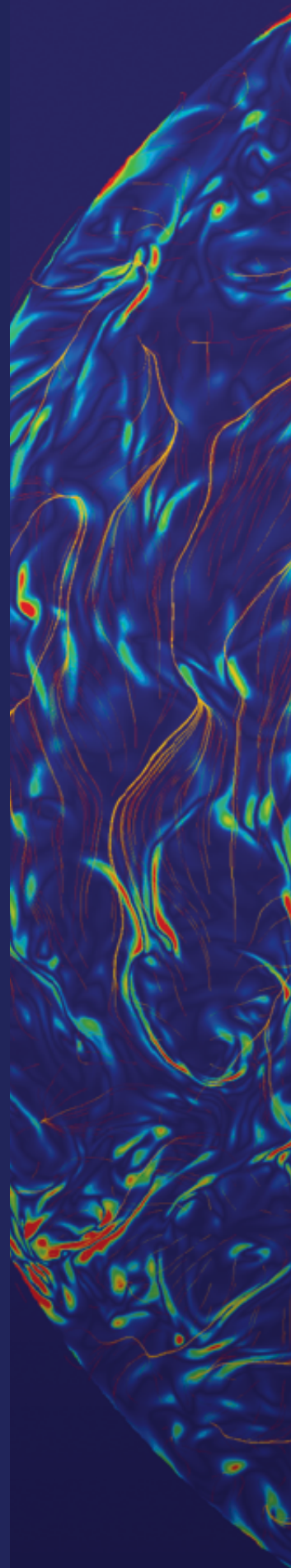
A snapshot of the boundary layer structure right at the heated bottom plate of a cylindrical cell for turbulent Rayleigh-Bénard convection in liquid sodium at a Rayleigh number of 10 million. The field lines of the skin friction field at the bottom plate are displayed in yellow. They provide a 2D blueprint of the velocity field near the plate. Colored contours correspond to the magnitude of the vorticity component taken in a horizontal plane near the velocity boundary layer. *Image: Joerg Schumacher, Technische Universitaet Ilmenau*

Awarding Compute Time on ALCF Resources

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

Researchers gain access to ALCF systems for computational science and engineering projects through competitive, peer-reviewed allocations programs supported by the DOE and Argonne.

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

APPLICATION PROGRAMS

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

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

ALLOCATION PROGRAMS

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

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

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

INCITE/ALCC BY DOMAIN

2018 INCITE allocated hours

3.78B

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

2018 ALCC allocated hours

1.86B

Biological Sciences	75	Million Core-Hours
Chemistry	56	
Computer Science	190	
Earth Science	109	
Energy Technologies	358	
Engineering	85	
Materials Science	367	
Physics	619	
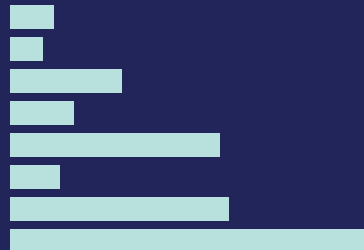
Note: ALCC data are from calendar year 2018.

Chemistry

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

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

Researchers have revealed a new technique to 'sew' two patches of crystals seamlessly together to create atomically thin fabrics. *Image: Saien Xie, Cornell University and the University of Chicago*

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

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

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

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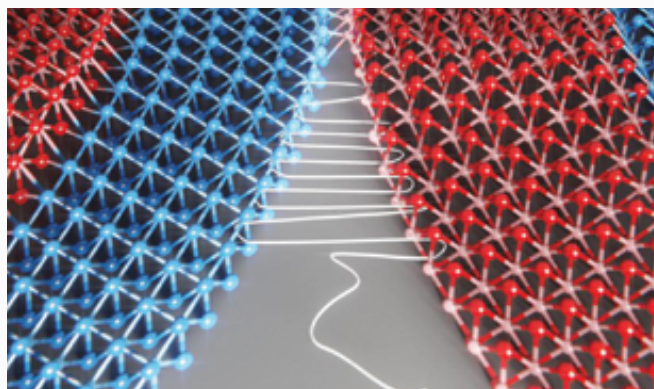
transition metal dichalcogenides for the heterostructures and superlattices. ALCF staff members assisted these efforts by helping to create ensemble jobs that run at full capability and by advising the optimization of Mira's nodal computational power.

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

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

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

Balsam: Workflow Manager and Edge Service for HPC Systems

PI   Thomas Uram, Taylor Childers
INST   Argonne National Laboratory
HOURS   DD, 250,000 Core-Hours

A schematic of the ATLAS deployment of Balsam on multiple computing resources to execute a workflow with alternating serial and parallel stage. *Image: Thomas Uram, Argonne National Laboratory*
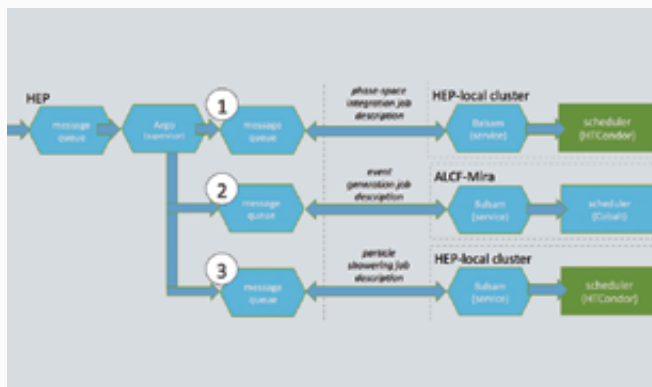
The ALCF's Balsam tool was originally developed as an "edge service," providing a simple, adaptable interface between high-performance computing (HPC) facilities and the job management systems operated by large-scale experimental science projects. ALCF researchers have further developed Balsam to serve as a workflow management tool that manages large-scale job campaigns for users, while diminishing the burden on the user and opening opportunities for optimizing how these jobs are submitted and executed.

CHALLENGE

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

APPROACH

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

RESULTS

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

More recently, the ALCF has released Balsam publicly to help researchers handle the cumbersome process of running many jobs across one or more HPC resources. In addition, the ALCF team has used Balsam to run ensemble jobs on more than 1,000 Theta nodes for ECP, ADSP, and ESP projects, involving quantum chemistry, materials science, and studies of hyperparameter optimization in deep learning (DeepHyper).

IMPACT

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

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

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

Earth Science

Accelerated Climate Modeling for Energy (ACME)

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

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

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

CHALLENGE

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

APPROACH

The team made extensive use of Theta to run the recently released ES3M code, which comprises component models for atmosphere, ocean, sea ice, and land. Sixty-four tasks were assigned to every node, each with two OpenMP threads so as to establish intranodal parallelism.

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

RESULTS

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

IMPACT

In addition to further advancing the predictive power of climate models and providing insight into the climatic effects of rapid changes in the earth's ice content, the ES3M simulations have the potential to answer how water resources and the hydrological cycle interact with the climate system on both local and global scales. Hurricane hindcast simulations performed for this project demonstrated the high fidelity with which extreme weather can be modeled, while exposing parametric weaknesses that need improvement.

Engineering

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

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

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

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

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

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

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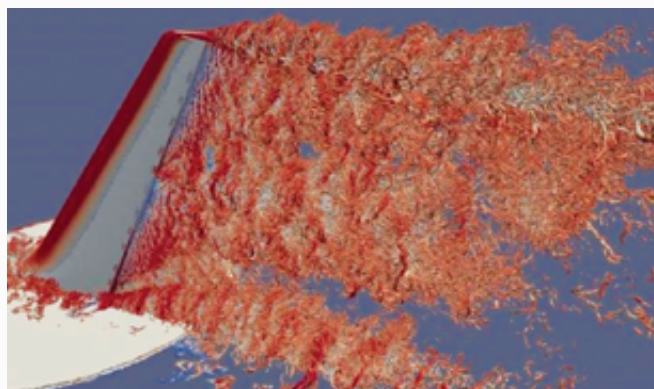
perform flight-scale simulations on Aurora once that system is available. The researchers are currently working on simulations featuring more complex turbulence conditions (corresponding to a Reynolds number of 700,000).

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

Engineering

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

PI   Pinaki Pal
INST   Argonne National Laboratory
HOURS   DD, 26.5 Million Core-Hours

Visualization from a high-fidelity simulation of a heavy-duty engine fueled with a straight-run gasoline performed on the Mira supercomputer by researchers from Argonne National Laboratory, Aramco Services Company: Aramco Research Center—Detroit, and Convergent Science Inc. *Image: Roberto Torelli and Joseph A. Insley, Argonne National Laboratory; Yuanjiang Pei, Aramco Services Company: Aramco Research Center—Detroit*

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

CHALLENGE

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

APPROACH

Running the CONVERGE code on Mira, the team performed a first-of-its-kind study using a high-fidelity simulation approach to optimize the fuel spray and combustion bowl geometry on a supercomputer. Model predictions were validated against experimental results generated using the production engine hardware. Large ensembles of simulations were then performed spanning a wide engine design space on Mira supercomputer, based on design of experiments (DOE) approach. Thereafter, the piston geometry and engine operating conditions were optimized in a staged manner using a response surface method. In an earlier project with Convergent Science, Inc., ALCF staff helped to optimize the CONVERGE code on Mira, resulting in a 100x speedup in I/O, an 8x improvement in load balance, and a 3.4x improvement in time-to-solution.
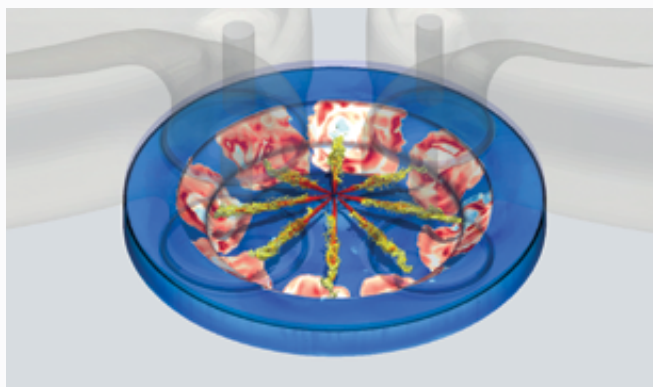
RESULTS

The team used Mira to simulate over 3,000 high-fidelity engine design combinations in a matter of days, covering four different operating conditions, 256 bowl geometries, multiple fuel injector-related configurations, and various start-of-injection scenarios. The team's simulations revealed design scenarios that showed an improvement in indicated specific fuel consumption of up to 6.3 percent while meeting the future low criteria pollutants standard. The computational study allowed the team to narrow down the best-performing scenarios to a specific set of piston and injector designs for further evaluation.

IMPACT

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

PUBLICATIONS

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

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

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

Materials Science

Data-Driven Molecular Engineering of Solar-Powered Windows

PI   Jacqueline Cole
INST   University of Cambridge
HOURS   ADSP, 117 Million Core-Hours
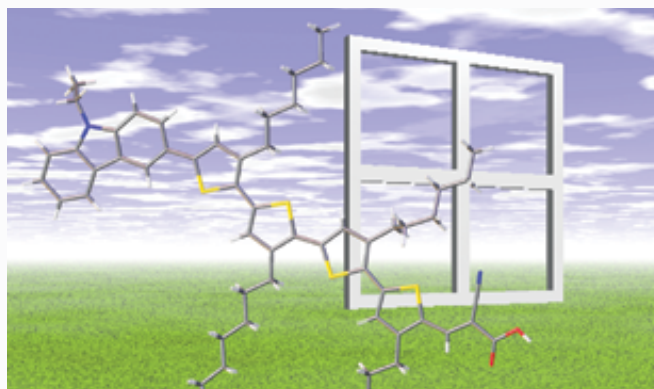
Abstract representation of solar-powered windows (including molecule designed for dye-sensitized solar cells). *Image: Jacqueline M. Cole, University of Cambridge*

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

CHALLENGE

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

APPROACH

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

RESULTS

Chemistry groups from around the world synthesized the six dyes predicted to have solar-cell prospects; co-sensitization experiments and materials characterization optimized them for solar-cell device fabrication and testing. These solar cells afforded photovoltaic outputs that were comparable to those of the industrial standard. These results have been published in *Advanced Energy Materials*, showcasing the power of data-driven materials discovery.

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

IMPACT

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

PUBLICATIONS

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

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

Materials Science

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

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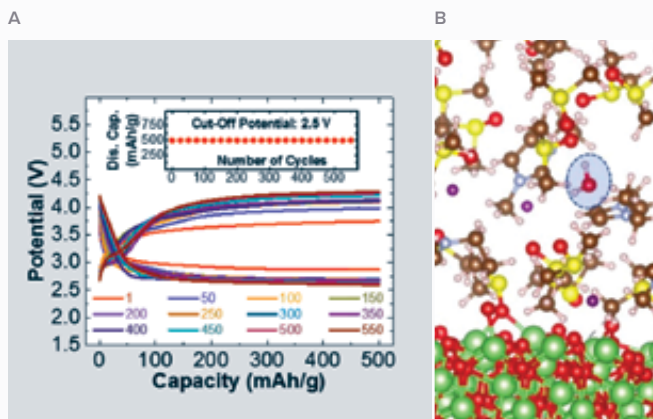HOURS   DD, 20 Million Core-Hours

A   B

(A) Voltage profiles for a Li-O$_2$ cell based on a MoS$_2$ cathode, ionic liquid/dimethyl sulfoxide electrolyte and lithium carbonate coated lithium anode with a cycle life of over 500 cycles in air. **(B)** Results of an *ab initio* molecular dynamics simulation using VASP of the electrolyte used in the Li-O$_2$ cell that helped explain its stability. *Image: Mohammad Asadi, et al.,* Nature

Previous experimental designs of Li-O$_2$ batteries have failed to operate in a true natural air environment due to the oxidation of lithium anodes by air components and to the production of undesirable byproducts on cathodes (a result of combining lithium ions with carbon dioxide and water vapor). These byproducts gum up the cathodes, which eventually become completely coated and nonfunctional during charge and discharge cycles. To circumvent this problem, these batteries have often relied on tanks of pure oxygen, which severely limits their practicality.

CHALLENGE

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

APPROACH

Using molecular dynamics simulations made possible by ALCF supercomputers , the team overcame these challenges by uniquely combining the three main components of any battery—anode, cathode, and electrolyte—to prevent anode oxidation and the buildup of battery-killing byproducts on the cathode, which permitted operation in a natural air environment. The researchers coated the lithium anode with a thin layer of lithium carbonate that selectively allowed the passage of lithium ions and prevented unwanted air components, such as nitrogen, from reaching the anode. The cathode employed a lattice structure with a molybdenum disulfide catalyst and a novel hybrid electrolyte made of ionic liquid and dimethyl

sulfoxide that helped facilitate Li-O$_2$ reactions, minimize reactions with ambient elements, and boosted the battery's efficiency. The complete architectural overhaul of the battery involved redesigning its every part to enable desirable reactions and block those that would kill the battery.

RESULTS

In a study published in *Nature*, the researchers reported a new design for a Li-O$_2$ battery cell that operates by reacting with air over numerous charge and discharge cycles. The battery was still functioning after a record-breaking 700 such cycles, which, being the first demonstration of a true Li-O$_2$ design, represents a significant advancement.

IMPACT

The new Li-O$_2$ cell architecture is a promising step toward engineering the next generation of lithium batteries with much higher specific energy density than lithium-ion batteries.

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

Modeling Electronic Stopping in Condensed Matter Under Ion Irradiation

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

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

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

CHALLENGE

Predictive modeling of electronic stopping processes has remained a great challenge for many decades because of the difficulties involved in accurately describing the quantum-mechanical excitation of electrons; however, recent innovations in first-principles calculation methodologies and massively parallel supercomputers have enabled accurate simulations of these processes at the atomistic level. The researchers now seek to further advance simulation capabilities so as to model complex systems like semiconductors and solvated DNA under various ion irradiations. A new challenge is to elucidate and correctly describe and understand the role of the (semi-)core electrons when matters are exposed to ion radiations beyond the typical proton radiation.

APPROACH

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

RESULTS

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

IMPACT

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

PUBLICATIONS

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

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

Materials Science

Predictive Simulations of Functional Materials

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

A   B

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

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

CHALLENGE

Since its successful isolation in 2004, monolayer graphene has been an object of intense research interest. Its many remarkable properties include Dirac cones, electronic band structures that describe unusual (and beneficial) electron transport. Monolayer graphene consists of a single layer of atoms (and is hence referred to as a two-dimensional material), the bonding structure of whose electron orbitals makes it extremely susceptible to environmental perturbation. Oxygen (O_2), due to its abundance and interactivity, is among the most important potential contaminants to study in depth.

APPROACH

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

QMC approaches solve the quantum many-body problem stochastically. They offer three key advantages over traditional density functional theories (DFTs): accuracy, efficiency, and, with only three possible sources of error, transparency. Moreover, they establish a strict upper-bound for total energy and exactly compute interatomic and -molecular interactions known as van der Waals forces, which DFT approaches can only approximate. As such, the
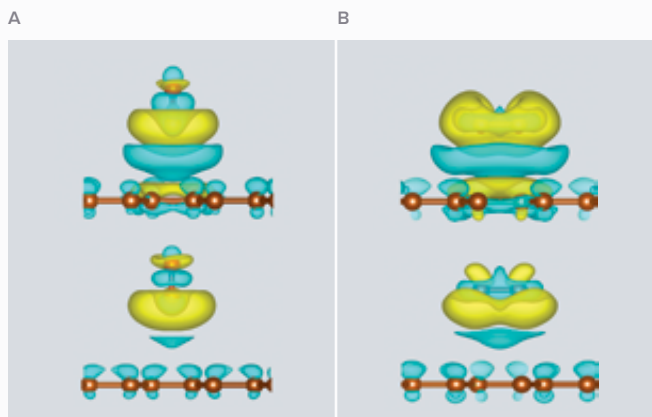
exceptional power of QMC made it ideal for modeling adsorption and diffusion of O_2 molecules on graphene surfaces.

RESULTS

Using simulations on Mira to examine various orientations of O_2 on the surface of graphene, the team was able to identify the most energetically stable modes. Furthermore, the results exposed the appreciable bias of DFT functionals toward under- and overestimations that van der Waals corrections entail.

IMPACT

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

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

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

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

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

Understanding Electronic Properties of Layered Perovskites with Extreme-Scale Computing

PI   Volker Blum
INST   Duke University
HOURS Theta ESP, 10 Million Core-Hours

(A) The supercell structure of a prototypical layered hybrid perovskite. Planar layers represent inorganic structures, while organic chains are ordered in diagonal arrangements. **(B)** Possible energy level schemes for an alternating organic-inorganic perovskite are shown with the overall band gap indicated by arrows and dashed lines. *Image: Chi Liu and Volker Blum, Duke University*
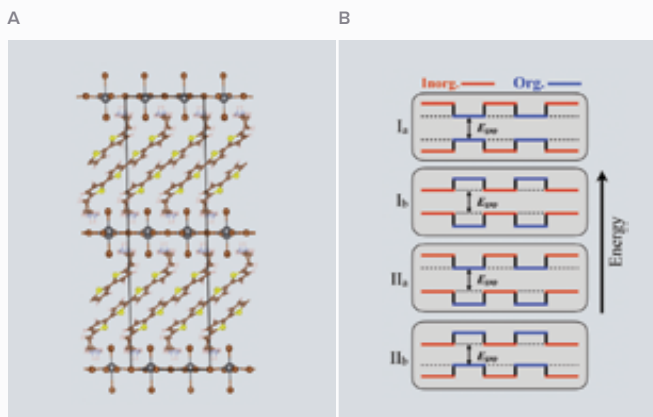
As with the flow of water, that of electrons can produce useful outcomes. It is therefore important to control the energy levels and flow of electrons and their counterparts, so-called holes, in high-quality electronic materials. One class of such materials are layered hybrid organic-inorganic perovskites (HOIPs), well-organized structures that combine organic and inorganic components (e.g., chains of doubly bonded molecular rings and ionic layers, respectively) to manipulate electron flow and the resulting light emission or absorption. Using ALCF supercomputing resources, Duke University researchers have demonstrated the possibility of understanding HOIPs as analogous to a system of "electron" and "hole" containers; this work could help create new materials with tunable optical properties.

CHALLENGE

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

APPROACH

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

and by scaling the density-functional code FHI-aims for use on the massively parallel Theta machine.

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

RESULTS

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

IMPACT

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

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

SCIENCE

Physics

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

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

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

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

CHALLENGE

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

APPROACH

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

RESULTS

Harvester and Yoda were integrated into the ATLAS production system, called PanDA, to run the ATLAS analysis framework on Theta. The ATLAS simulation process is composed of three steps: event generation, simulation, and reconstruction. This work was done in parallel and depended on software containerization given the different
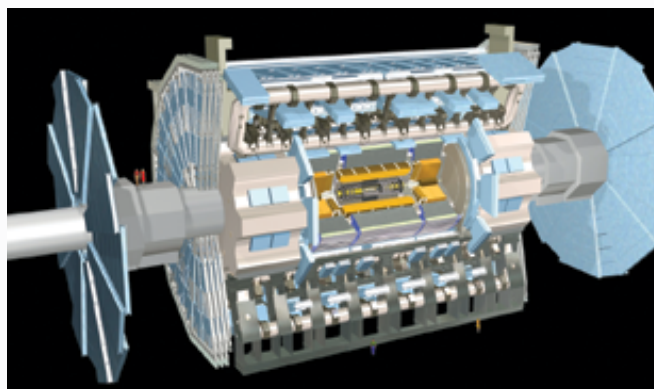
physics releases and libraries required for each step. Over 37 million events have been simulated on Theta, with many validating the workflow and chip architecture to ensure physics results produced agree with those from previous systems. The team's established functionality has permitted the generation of custom datasets that will be used to study machine learning techniques that could replace custom algorithms in the reconstruction.

IMPACT

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

Physics

Global Radiation MHD Simulations of Massive Star Envelopes

PI   Lars Bildsten
INST   University of California, Santa Barbara
HOURS   INCITE, 60 Million Core-Hours
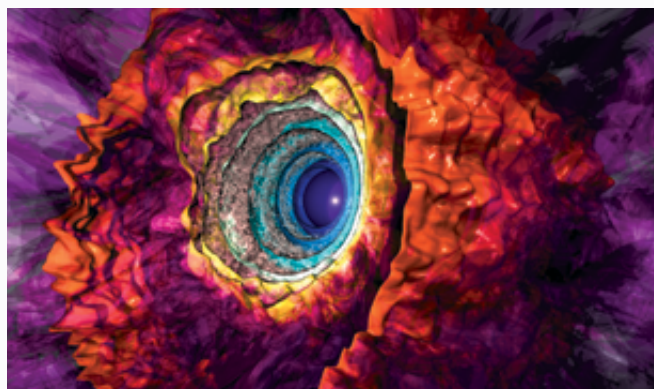
Global radiation hydrodynamic simulation of massive star envelope.
Image: Joseph A. Insley, Argonne National Laboratory

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

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

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

RESULTS
The researchers repeated two of the first year's global simulations with different metallicities to study the effects thereof on envelope structures and mass-loss rate, detailing their findings in *Nature*. It was discovered that increased metallicity produces stronger turbulence and causes a larger

helium opacity peak, leading to stronger winds and larger amplitude variability. Reduced metallicity fails to produce a strong helium opacity peak, reducing the outflow rate from massive stars.

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

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

Physics

Multiscale Physics of the Ablative Rayleigh-Taylor Instability

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

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

The Rayleigh-Taylor Instability (RTI), a ubiquitous phenomenon that occurs when a heavy fluid is accelerated against a light fluid, is a major obstacle to current efforts to realize inertial confinement fusion (ICF) as an energy source. Researchers from the University of Rochester are using ALCF resources to study, via simulations, how ablation (mass evaporation due to a heat source) affects RTI evolution. In doing so they hope to elucidate RTI's role in ICF implosions.
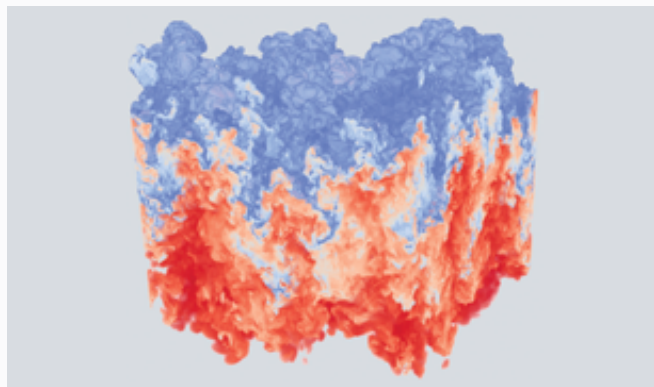
CHALLENGE
RTI, which has hindered yields in ICF, describes the interfacial instability of a dense fluid atop a lighter fluid when a downward acceleration field is present. It can be viewed as a given system's attempt to reduce its potential energy by lowering its center of mass, manifested in the formation of rising bubbles and sinking spikes in the light and heavy fluids, respectively. Such flows further amplify fluctuations and mixing, which leads to extreme nonlinearity.

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

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

scaled to one third of the Mira system (roughly 260,000 cores) for the largest simulations.

RESULTS
The researchers discovered that, contrary to current modeling practices, any length-scale in ablative RTI can be destabilized if the initial perturbation is sufficiently large. The vast dynamic range afforded by their simulations provided numerical evidence for the optimal way to analyze length-scales in highly nonlinear flows with significant density variations. The team detailed these findings in papers published in *Physical Review Letters*, *Physical Review E*, and *Physical Review Fluids*.
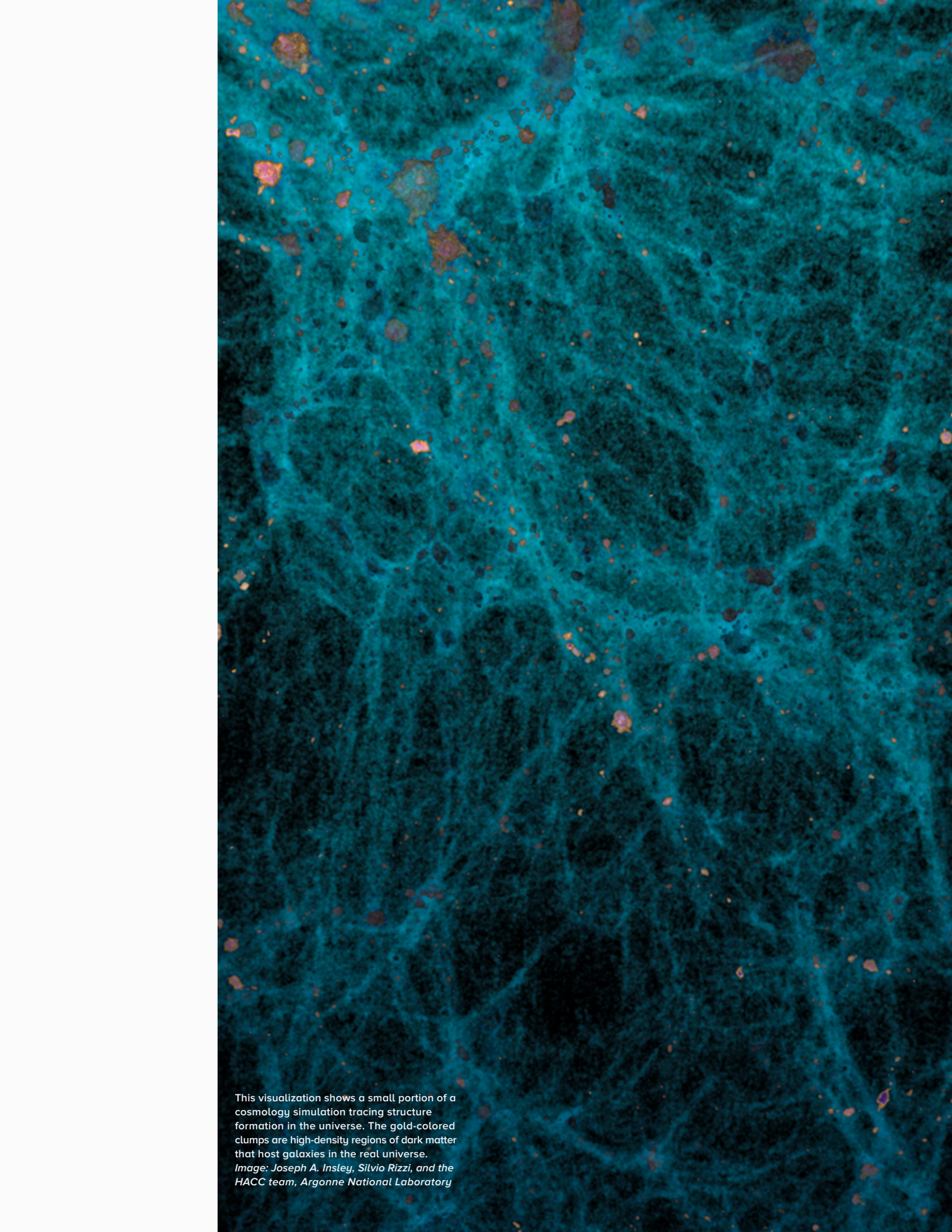
IMPACT
Beyond bringing nuclear fusion closer to realization as a viable and virtually limitless energy source, this work carries important ramifications for modeling implosion physics, astrophysics, oceanic flows, and combustion science.

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

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

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

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

ALCF Projects

2018 INCITE Projects

BIOLOGICAL SCIENCES

Biophysical Principles of Functional Synaptic Plasticity in the Neocortex

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

The Free Energy Landscapes Governing Membrane Protein Function

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

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

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

CHEMISTRY

Advancing Design and Structure Prediction of Proteins and Peptides

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

High-Accuracy Quantum Approaches for Predictions of Catalysis on Solids

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

COMPUTER SCIENCE

Performance Evaluation and Analysis Consortium (PEAC) End Station

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

EARTH SCIENCE

Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations

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

High-Resolution Climate Change Simulations with the CESM

PI	Gerald Meehl
INST	NCAR
HOURS	264 Million Core-Hours

Accelerated Climate Modeling for Energy (ACME)

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

ENERGY TECHNOLOGIES

Towards Predictive Exascale Wind Farm Simulations

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

ENGINEERING

Multiscale Physics of the Ablative Rayleigh-Taylor Instability

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

Crystal Plasticity from First Principles

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

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

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

High-Accuracy LES of a Multistage Compressor Using Discontinuous Galerkin

PI	Koen Hillewaert
INST	Cenaero
HOURS	78 Million Core-Hours

Large-Eddy Simulation of a Commercial Transport Aircraft Model

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

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

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

Convective Turbulence in Liquid Sodium

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

MATERIALS SCIENCE

Modeling Electronic Stopping in Condensed Matter Under Ion Irradiation

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

Predictive Simulations of Functional Materials

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

Materials and Interfaces for Organic and Hybrid Photovoltaics

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

Petascale Simulations for Layered Materials Genome

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

PHYSICS

Global Radiation MHD Simulations of Massive Star Envelopes

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

Collider Physics at the Precision Frontier

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

High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics

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

Extreme-Scale Simulation of Supernovae and Magnetars from Realistic Progenitors

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

Multiscale Modeling of Magnetic Reconnection in Space and Laboratory Plasmas

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

Kinetic Simulation of FRC Stability and Transport

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

Nuclear Structure and Nuclear Reactions

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

Lattice QCD

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

Hadron Structure from Lattice QCD

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

PICSSAR

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

Astrophysical Particle Accelerators: Magnetic Reconnection and Turbulence

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

2017–2018 ALCC Projects

BIOLOGICAL SCIENCES

Multiscale Simulations of Hematological Disorders

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

Protein-Protein Recognition and HPC Infrastructure

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

CHEMISTRY

Quantum Monte Carlo Computations of Chemical Systems

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

Spin-Forbidden Catalysis on Metal-Sulfur Proteins

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

COMPUTER SCIENCE

ECP Consortium for Exascale Computing

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

Portable Application Development for Next-Generation Supercomputer Architectures

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

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications

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

EARTH SCIENCE

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

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

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

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

ENERGY TECHNOLOGIES

High-Fidelity Numerical Simulation of Wire-Wrapped Fuel Assemblies

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

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

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

ENGINEERING

Non-Boussinesq Effects on Buoyancy-Driven Variable Density Turbulence

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

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

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

MATERIALS SCIENCE

Computational Engineering of Electron-Vibration Coupling Mechanisms

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

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

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

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

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

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

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

PHYSICS

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

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

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

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

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

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

Studying Astrophysical Particle Acceleration in HED Plasmas

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

Extreme-Scale Simulations for Multi-Wavelength Cosmology Investigations

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

Nuclear Spectra with Chiral Forces

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

Nucleon Structure and Electric Dipole Moments with Physical Chirally Symmetric Quarks

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

2018–2019 ALCC Projects

CHEMISTRY

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

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

COMPUTER SCIENCE

Portable Application Development for Next-Generation Supercomputer Architectures

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

Demonstration of the Scalability of Programming Environments by Simulating Multiscale Applications

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

EARTH SCIENCE

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

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

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

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

ENERGY TECHNOLOGIES

Multiphase Flow Simulations of Nuclear Reactor Flows

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

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

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

HPC4EnergyInnovation ALCC End-Station

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

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

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

ENGINEERING

Analysis and Mitigation of Dynamic Stall in Energy Machines

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

MATERIALS SCIENCE

Large-Scale Simulations of Heterogeneous Materials for Energy Conversion Applications

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

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

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

Impact of Grain Boundary Defects on Hybrid Perovskite Solar Absorbers

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

Predictive Modeling and Machine Learning for Functional Nanoporous Materials

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

Modeling Fusion Plasma Facing Components

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

PHYSICS

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

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

Emulating the Universe

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

Scaling LHC Proton-Proton Collision Simulations in the ATLAS Detector

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

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

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

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

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

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

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

ALCF Data Science Program

Massive Hyperparameter Searches on Deep Neural Networks Using Leadership Systems

PI   Pierre Baldi
INST   University of California, Irvine

Enabling Multiscale Physics for Industrial Design Using Deep Learning Networks

PI   Rathakrishnan Bhaskaran
INST   GE Global Research

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

PI   Taylor Childers
INST   Argonne National Laboratory

Data-Driven Molecular Engineering of SolarPowered Windows

PI   Jacqueline Cole
INST   University of Cambridge

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

PI   Fabien Delalondre
INST   Ecole Federale Polytechnique
          de Lausanne

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

PI   Doga Gursoy
INST   Argonne National Laboratory

Realistic Simulations of the LSST Survey at Scale

PI   Katrin Heitmann
INST   Argonne National Laboratory

Constructing and Navigating Polymorphic Landscapes of Molecular Crystals

PI   Alexandre Tkatchenko
INST   University of Luxembourg

Aurora Early Science Program

Extending Moore's Law Computing with Quantum Monte Carlo

PI   Anouar Benali
INST   Argonne National Laboratory

Exascale Computational Catalysis

PI   David Bross
INST   Argonne National Laboratory

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI   C.S. Chang
INST   Princeton Plasma Physics Laboratory

Machine Learning for Lattice Quantum Chromodynamics

PI   William Detmold
INST   Massachusetts Institute of Technology

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

PI   Thom Dunning
INST   Pacific Northwest National Laboratory

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI   Nicola Ferrier
INST   Argonne National Laboratory

Dark Sky Mining

PI   Salman Habib
INST   Argonne National Laboratory

Extreme-Scale Cosmological Hydrodynamics

PI   Katrin Heitmann
INST   Argonne National Laboratory

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI   Kenneth Jansen
INST   University of Colorado Boulder

Extreme-Scale Unstructured Adaptive CFD

PI   Kenneth Jansen
INST   University of Colorado Boulder

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

PI   Noa Marom
INST   Carnegie Mellon University

Simulating and Learning in the ATLAS Detector at the Exascale

PI   James Proudfoot
INST   Argonne National Laboratory

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

PI   Amanda Randles
INST   Duke University
          Oak Ridge National Laboratory

Virtual Drug Response Prediction

PI   Rick Stevens
INST   Argonne National Laboratory

Accelerated Deep Learning Discovery in Fusion Energy Science

PI   William Tang
INST   Princeton Plasma Physics Laboratory

2018 Director's Discretionary Projects
The following list provides a sampling of the many Director's Discretionary projects at the ALCF.

BIOLOGICAL SCIENCES

Computational Analysis of Brain Connectomes for Alzheimer's Disease

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

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

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

Cancer Workflow Toolkit

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

CHEMISTRY

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

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

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

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

COMPUTER SCIENCE

System Software to Enable Data-Intensive Science

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

MPICH - A High-Performance and Widely Portable MPI Implementation

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

EARTH SCIENCE

Simulating Global Terrestrial Carbon Sequestration and Carbon Transport to Aquatic Ecosystems

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

ENGINEERING

Simulation of Supersonic Combustion

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

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

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

Data Analysis of Turbulent Channel Flow at High Reynolds Number

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

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

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

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

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

HPC4Mfg: Modeling Paint Behavior During Rotary Bell Atomization

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

Full Core PWR Simulation Using 3D Method of Characteristics

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

MATERIALS SCIENCE

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

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

Rational Design of Ultrastrong Composites

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

Phase Transitions in Water-Ice-Vapor System

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

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

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

2T-MD Model Simulations of High Energy Ion Irradiation

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

PHYSICS

Scalable Reconstruction of X-ray Scattering Imaging for Nanomaterials

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

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

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

MARS Energy Deposition and Neutrino Flux Simulations

PI	Nikolai Mokhov
INST	Fermilab
HOURS	18 Million Core-Hours

Scaling and Performance Enhancement of an Astrophysical Plasma Code

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

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

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

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

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

Quantum Monte Carlo Modeling of Strongly Correlated Electronic Systems

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

ALCF Publications

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

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

January

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

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

Balin, R., and K. E. Jansen. "A Comparison of RANS, URANS, and DDES for High Lift Systems from HiLiftPW-3," *2018 AIAA Aerospace Sciences Meeting, AIAA SciTech Forum* (January 2018), Kissimmee, Florida, AIAA. doi:10.2514/6.2018-1254.

Chard, K. E. Dart, I. Foster, D. Shifflett, S. Tuecke, and J. Williams. "The Modern Research Data Portal: A Design Pattern for Networked, Data-Intensive Science," *PeerJ Computer Science* (January 2018), PeerJ. doi:10.7717/peerj-cs.144.

Gaiduk, A. P., T. A. Pham, M. Govoni, F. Paesani, and G. Galli. "Electron Affinity of Water," *Nature Communications* (January 2018), Springer Nature. doi:10.1038/s41467-017-02673-z.

Guenther, J., R. Bellwied, S. Borsanyi, Z. Fodor, A. Pasztor, C. Ratti, S. D. Katz, and K. Szabo. "Recent Lattice QCD Results at Non-Zero Baryon Densities," *Proceedings of Science* (January 2018), Sissa Medialab. doi:10.22323/1.311.0032.

Hong, S., A. Krishnamoorthy, C. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta. "A Reactive Molecular Dynamics Study of Atomistic Mechanisms During Synthesis of MoS_2 Layers by Chemical Vapor Deposition," *MRS Advances* (January 2018), Cambridge University Press. doi:10.1557/adv.2018.67.

Ichibha, T., K. Hongo, I. Motochi, N. W. Makau, G. O. Amolo, and R. Maezono. "Adhesion of Electrodes on Diamond (111) Surface: A DFT Study," *Diamond and Related Materials* (January 2018), Elsevier. doi:10.1016/j.diamond.2017.12.008.

Kumazoe, H., A. Krishnamoorthy, L. Bassman, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. "Photo-Induced Contraction of Layered Materials," *MRS Advances* (January 2018), Cambridge University Press. doi:10.1557/adv.2018.127.

Kruse, M. and H. Finkel. "A Proposal for Loop-Transformation Pragmas," *Evolving OpenMP for Evolving Architectures* (January 2018), Barcelona, Spain, Springer. doi:10.1007/978-3-319-98521-3_3.

Li, Y., K. Nomura, J. Insley, V. Morozov, K. Kumaran, N. Romero, W. A. Goddard III, R. Kalia, A. Nakano, and P. Vashishta. "Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis," *Computing in Science and Engineering* (January 2018), IEEE. doi:10.1109/MCSE.2018.110150043.

Lockwood, G. K., S. Snyder, G. Brown, K. Harms, P. Carns, and N. J. Wright. "TOKIO on ClusterStor: Connecting Standard Tools to Enable Holistic I/O Performance Analysis," *Proceedings of the 2018 Cray User Group* (January 2018), Cray User Group.

Macridin, A. A. Burov, E. Stern, J. Amundson, and P. Spentzouris. "Parametric Landau Damping of Space Charge Modes," *Physical Review Accelerators and Beams* (January 2018), APS. doi:10.1103/physrevaccelbeams.21.011004.

O'Connor, E. and S. Couch. "Two-Dimensional Core-Collapse Supernova Explosions Aided by General Relativity with Multidimensional Neutrino Transport," *The Astrophysical Journal* (January 2018), IOP Publishing. doi:10.3847/1538-4357/aaa893.

Parotto, Paolo. "Parametrized Equation of State for QCD from 3D Ising Model," *Proceedings of Science* (January 2018), Sissa Medialab. doi:10.22323/1.311.0036.

January

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

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

Balin, R., and K. E. Jansen. "A Comparison of RANS, URANS, and DDES for High Lift Systems from HiLiftPW-3," *2018 AIAA Aerospace Sciences Meeting, AIAA SciTech Forum* (January 2018), Kissimmee, Florida, AIAA. doi:10.2514/6.2018-1254.

Chard, K. E. Dart, I. Foster, D. Shifflett, S. Tuecke, and J. Williams. "The Modern Research Data Portal: A Design Pattern for Networked, Data-Intensive Science," *PeerJ Computer Science* (January 2018), PeerJ. doi:10.7717/peerj-cs.144.

Gaiduk, A. P., T. A. Pham, M. Govoni, F. Paesani, and G. Galli. "Electron Affinity of Water," *Nature Communications* (January 2018), Springer Nature. doi:10.1038/s41467-017-02673-z.

Guenther, J., R. Bellwied, S. Borsanyi, Z. Fodor, A. Pasztor, C. Ratti, S. D. Katz, and K. Szabo. "Recent Lattice QCD Results at Non-Zero Baryon Densities," *Proceedings of Science* (January 2018), Sissa Medialab. doi:10.22323/1.311.0032.

Hong, S., A. Krishnamoorthy, C. Sheng, R. K. Kalia, A. Nakano, and P. Vashishta. "A Reactive Molecular Dynamics Study of Atomistic Mechanisms During Synthesis of MoS_2 Layers by Chemical Vapor Deposition," *MRS Advances* (January 2018), Cambridge University Press. doi:10.1557/adv.2018.67.

Ichibha, T., K. Hongo, I. Motochi, N. W. Makau, G. O. Amolo, and R. Maezono. "Adhesion of Electrodes on Diamond (111) Surface: A DFT Study," *Diamond and Related Materials* (January 2018), Elsevier. doi:10.1016/j.diamond.2017.12.008.

Kumazoe, H., A. Krishnamoorthy, L. Bassman, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. "Photo-Induced Contraction of Layered Materials," *MRS Advances* (January 2018), Cambridge University Press. doi:10.1557/adv.2018.127.

Kruse, M. and H. Finkel. "A Proposal for Loop-Transformation Pragmas," *Evolving OpenMP for Evolving Architectures* (January 2018), Barcelona, Spain, Springer. doi:10.1007/978-3-319-98521-3_3.

Li, Y., K. Nomura, J. Insley, V. Morozov, K. Kumaran, N. Romero, W. A. Goddard III, R. Kalia, A. Nakano, and P. Vashishta. "Scalable Reactive Molecular Dynamics Simulations for Computational Synthesis," *Computing in Science and Engineering* (January 2018), IEEE. doi:10.1109/MCSE.2018.110150043.

Lockwood, G. K., S. Snyder, G. Brown, K. Harms, P. Carns, and N. J. Wright. "TOKIO on ClusterStor: Connecting Standard Tools to Enable Holistic I/O Performance Analysis," *Proceedings of the 2018 Cray User Group* (January 2018), Cray User Group.

Macridin, A. A. Burov, E. Stern, J. Amundson, and P. Spentzouris. "Parametric Landau Damping of Space Charge Modes," *Physical Review Accelerators and Beams* (January 2018), APS. doi:10.1103/physrevaccelbeams.21.011004.

O'Connor, E. and S. Couch. "Two-Dimensional Core-Collapse Supernova Explosions Aided by General Relativity with Multidimensional Neutrino Transport," *The Astrophysical Journal* (January 2018), IOP Publishing. doi:10.3847/1538-4357/aaa893.

Parotto, Paolo. "Parametrized Equation of State for QCD from 3D Ising Model," *Proceedings of Science* (January 2018), Sissa Medialab. doi:10.22323/1.311.0036.

Qiu, J. X., H. J. Yoon, P. A. Fearn, and G. D. Tourassi. "Deep Learning for Automated Extraction of Primary Sites from Cancer Pathology Reports," *IEEE Journal of Biomedical and Health Informatics* (January 2018), IEEE. doi:10.1109/JBHI.2017.2700722.

Rakhno, I. L., N. V. Mokhov, I. S. Tropin, and D. Ene. "Activation Assessment of the Soil around the ESS Accelerator Tunnel," *Journal of Physics Conference Series* (January 2018), IOP Publishing. doi:10.1088/1742-6596/1046/1/012020.

Rodrigo, G. P., P.-O. Östberg, E. Elmroth, K. Antypas, R. Gerber, and L. Ramakrishnan. "Towards Understanding HPC Users and Systems: A NERSC Case Study," *Journal of Parallel and Distributed Computing* (January 2018), Elsevier. doi:10.1016/j.jpdc.2017.09.002.

Sebille, E. van, S. M. Griffies, R. Abernathey, T. P. Adams, P. Berloff, A. Biastoch. B. Blanke, E. P. Chassignet, Y. Cheng, C. J. Cotter, E. Deleersnijder, K. Döös, H. F. Drake, S. Drijfhout, S. F. Gary, A. W. Heemink, J. Kjellsson, I. M. Koszalka, M. Lange, C. Lique, G. A. MacGilchrist, R. Marsh, C. G. Mayorga Adame, R. McAdam, F. Nencioli, C. B. Paris, M. D. Piggott, J. A. Polton, S. Rühs, S. H.A.M. Shah, M. D. Thomas, J. Wang, P. J. Wolfram, L. Zanna, and J. D. Zika. "Lagrangian Ocean Analysis: Fundamentals and Practices," *Ocean Modelling* (January 2018), Elsevier. doi:10.1016/j.ocemod.2017.11.008.

Suh, D. B. K. Radak, C. Chipot, and B. Roux. "Enhanced Configurational Sampling with Hybrid Non-Equilibrium Molecular Dynamics-Monte Carlo Propogator," *The Journal of Chemical Physics* (January 2018), AIP. doi:10.1063/1.5004154.

Yu, V. W., F. Corsetti, A. Garcia, W. P. Huhn, M. Jacquelin, W. Jia, B. Lange, L. Lin, J. Lu, W. Mi, A. Seifitokaldani, Á. Vázquez-Mayagoitia, C. Yang, H. Yang, and V. Blum. "ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers," *Computer Physics Communications* (January 2018), Elsevier. doi:10.1016/j.cpc.2017.09.007.

Zhang, H., R. Betti, V. Gopalaswamy, R. Yan, and H. Aluie. "Nonlinear Excitation of the Ablative Rayleigh-Taylor Instability for All Wave Numbers," *Physical Review E* (January 2018), APS. doi:10.1103/physreve.97.011203.

Zimmerman, N. E. R., D. C. Hannah, Z. Rong, M. Liu, G. Ceder, M. Haranczyk, and K. A. Persson. "Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite0Size Ion Models," *The Journal of Physical Chemistry Letters* (January 2018), ACS. doi:10.1021/acs.jpclett.7b03199.

February

Apte, A. V. Kochat, P. Rajak, A. Krishnamoorthy, P. Manimunda, J. A. Hachtel, J. C. Idrobo, S. A. S. Amanulla, P. Vashishta, A. Nakano, R. K. Kalia, C. S. Tiwary, and P. M. Ajayan. "Structural Phase Transformation in Strained Monolayer $MoWSe_2$ Alloy," *ACS Nano* (February 2018), ACS. doi:10.1021/acsnano.8b00248.

Cherukara, M. J., D. S. Schulmann, K. Sasikumar, A. J. Arnold, H.Chan, S. Sadasivam, W. Cha, J. Maser, S. Das, S. K. R. S. Sankaranarayanan, and R. J. Harder. "Three-Dimensional Integrated X-ray Diffraction Imaging of a Native Strain in Multi-Layered WSe_2," *Nano Letters* (February 2018), ACS. doi:10.1021/acs.nanolett.7b05441.

Cole, J. M. "Data-Driven Molecular Engineering of Solar Powered Windows," *Computing in Science and Engineering* (February 2018), IEEE. doi:10.1109/MCSE.2018.011111129.

Curtis, F., X. Li, Á. Vázquez-Mayagoitia, S. Bhattacharya, L. M. Ghiringhelli, and N. Marom. "GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction," *Journal of Chemical Theory and Computation* (February 2018), ACS. doi:10.1021/acs.jctc.7b01152.

DiStasio Jr., R. A., G. Zhang, F. H. Stillinger, and S. Torquato. "Rational Design of Stealthy Hyperuniform Two-Phase Media with Tunable Order," *Physical Review E* (February 2018), APS. doi:10.1103/physreve.97.023311.

Ekström, A., G. Hagen, T. D. Morris, T. Papenbrock, and P. D. Schwartz. "Δ Isobars and Nuclear Saturation," *Physical Review C* (February 2018), APS. doi:10.1103/PhysRevC.97.024332.

Feng, J., and I. A. Bolotnov. "Effect of the Wall Presence on the Bubble Interfacial Forces in a Shear Flow Field," *International Journal of Multiphase Flow* (February 2018), Elsevier. doi:10.1016/j.ijmultiphaseflow.2017.10.004.

Fetisov, E. O., M. S. Shah, C. Knight, M. Tsapatsis, and J. I. Siepmann. "Understanding the Reactive Adsorption of H_2S and CO_2 in Sodium-Exchanged Zeolites," *ChemPhysChem* (February 2018), Wiley-VCH. doi:10.1002/cphc.201700993.

Geada, I. L., H. Ramezani-Dakhel, T. Jamil, M. Sulpizi, and H. Heinz. "Insight into Induced Charges at Metal Surfaces and Biointerfaces Using a Polarizable Lennard-Jones Potential," *Nature Communications* (February 2018). Springer Nature. doi:10.1038/s41467-018-03137-8.

Govoni, M., and G. Galli. "GW100: Comparison of Methods and Accuracy of Results Obtained with the WEST Code," *J* (February 2018), ACS. doi:10.1021/acs.jctc.7b00952.

Hammond, K. D., S. Blondel, L. Hu, D. Maroudas, and B. D. Wirth. "Large-Scale Atomistic Simulations of Low-Energy Helium Implantation into Tungsten Single Crystals," *Acta Materialia* (February 2018), Elsevier. doi:10.1016/j.actamat.2017.09.061.

Kostuk, M., T. D. Uram, T. Evans, D. M. Orlov, M. E. Papka, and D. Schissel. "Automatic Between-Pulse Analysis of DIII-D Experimental Data Performed Remotely on a Supercomputer at Argonne Leadership Computing Facility," *Fusion Science and Technology* (February 2018), Taylor and Francis Group. doi:10.1080/15361055.2017.1390388.

Li, Z., X. Bian, Y.-H. Tang, and G. E. Karniadakis. "A Dissipative Particle Dynamics Method for Arbitrarily Complex Geometries," *Journal of Computational Physics* (February 2018), Elsevier. doi:10.1016/j.jcp.2017.11.014.

Lovato, A., S. Gandolfi, J. Carlson, E. Lusk, S. C. Pieper, and R. Schiavilla. "Quantum Monte Carlo Calculation of Neutral-Current ν-12C Inclusive Quasielastic Scattering," *Physical Review C* (February 2018), APS. doi:10.1103/PhysRevC.97.022502.

Parotto, P. "Constraints on the Hadronic Spectrum from Lattice QCD," *Journal of Physics: Conference Series* (February 2018), IOP Publishing. doi:10.1088/1742-6596/1024/1/012018.

Piarulli, M., A. Baroni, L. Girlanda, A. Kievsky, A. Lovato, E. Lusk, L. E. Marcucci, S. C. Pieper, R. Schiavilla, M. Viviani, and R. B. Wiringa. "Light-Nuclei Spectra from Chiral Dynamics," *Physical Review Letters* (February 2018), APS. doi:10.1103/PhysRevLett.120.052503.

Raju, M. K., J. N. Orce, P. Navrátil, G. C. Ball, T. E. Drake, S. Triambak, G. Hackman, C. J. Pearson, K. J. Abrahams, E. H. Akakpo, H. Al Falou, R. Churchman, D. S. Cross, M. K. Djongolov, N. Erasmus, P. Finlay, A. B. Garnsworthy, P. E. Garrett, D. G. Jenkins, R. Kshetri, K. G. Leach, S. Masango, D. L. Mavela, C. V. Mehl, M. J. Mokgolobotho, C. Ngwetsheni, G. G. O'Neill, E. T. Rand, S. K. L. Sjue, C. S. Sumithrarachchi, C. E. Svensson, E. R. Tardiff, S. J. Williams, and J. Wong. "Reorientation-Effect Measurement of the First 2+ State in ^{12}C: Confirmation of Oblate Deformation," *Physical Letters B* (February 2018), Elsevier. doi:10.1016/j.physletb.2017.12.009.

Ratcliff, L. E., A. Degomme, J. A. Flores-Livas, S. Goedecker, and L. Genovese. "Affordable and Accurate Large-Scale Hybrid-Functional Calculations on GPU-Accelerated Supercomputers," *Journal of Physics: Condensed Matter* (February 2018), IOP Publishing. doi:10.1088/1361-648X/aaa8c9.

Ratti, C. "Lattice QCD Results on Chemical Freeze-Out," *17th International Conference on Strangeness in Quark Matter* (February 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817105002.

Scheurer, M., P. Rodenkirch, M. Siggel, R. C. Bernardi, K. Schulten, E. Tajkhorshid, and T. Rudack. "PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations," *Biophysical Journal* (February 2018), Cell Press. doi:10.1016/j.bpj.2017.12.003.

Smith, C. W., M. Rasquin, D. Ibanez, K. E. Jansen, and M. S. Shephard. "Improving Unstructured Mesh Partitions for Multiple Criteria Using Mesh Adjacencies," *SIAM Journal on Scientific Computing* (February 2018), SIAM. doi:10.1137/15m1027814.

Tzeferacos, P., A. Rigby, A. F. A. Bott, A. R. Bell, R. Bingham, A. Casner, F. Cattaneo, E. M. Churazov, J. Emig, F. Fiuza, C. B. Forest, J. Foster, C. Graziani, J. Katz, M. Koenig, C.-K. Li, J. Meinecke, R. Petrasso, H.-S. Park, B. A. Remington, J. S. Ross, D. Ryu, D. Ryutov, T. G. White, B. Reville, F. Miniati, A. A. Schekochihin, D. Q. Lamb, D. H. Froula, and G. Gregori. "Laboratory Evidence of Dynamo Amplification of Magnetic Fields in a Turbulent Plasma," *Nature Communications* (February 2018), Springer Nature. doi:10.1038/s41467-018-02953-2.

Tramm, J. R., K. S. Smith, B. Forget, and A. R. Siegel. "ARRC: A Random Ray Neutron Transport Code for Nuclear Reactor Simulation," *Annals of Nuclear Energy* (February 2018), Elsevier. doi:10.1016/j.anucene.2017.10.015.

Wang, D., E.-S. Jung, R. Kettimuthu, I. Foster, D. J. Foran, and M. Parashar. "Supporting Real-Time Jobs on the IBM Blue Gene/Q: Simulation-Based Study," *Job Scheduling Strategies for Parallel Processing* (February 2018), Springer Nature. doi:10.1007/978-3-319-77398-8_5.

Whiteman, P. J., J. F. Schultz, Z. D. Porach, H. Chen, and N. Jiang. "Dual Binding Configurations of Subphthalocyanine on Ag(100) Substrate Characterized by Scanning Tunneling Microscopy, Tip-Enhanced Raman Spectroscopy, and Density Functional Theory," *The Journal of Physical Chemistry C* (February 2018), ACS. doi:10.1021/acs.jpcc.7b12068.

Yang, X., V. De Andrade, W. Scullin, E. L. Dyer, N. Kasthuri, F. De Carlo, and D. Gursoy. "Low-Dose X-ray Tomography through a Deep Convolutional Neural Network," *Scientific Reports* (February 2018), Springer Natuer. doi:10.1038/s41598-018-19426-7.

Yazdani, A., H. Li, M. R. Bersi, P. Di Achille, J. Insley. J. D. Humphrey, and G. E. Karniadakis. "Data-Driven Modeling of Hemodynamics and Its Role on Thrombus Size and Shape in Aortic Dissections," *Scientific Reports* (February 2018), Springer Nature. doi:10.1038/s41598-018-20603-x.

Zhang, K., A. Guliani, S. Ogrenci-Memik, G. Memik, K. Yoshii, R. Sankaran, and P. Beckman. "Machine Learning-Based Temperature Prediction for Runtime Thermal Management Across System Components," *IEEE Transactions on Parallel and Distributed Systems* (February 2018), IEEE. doi:10.1109/tpds.2017.2732951.

Zhang, L., Q. Zheng, Y. Xie, Z. Lan, O. V. Prezhdo, W. A. Saidi, and J. Zhao. "Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors," *Nano Letters* (February 2018), ACS. doi:10.1021/acs.nanolett.7b03933.

Zhao, L., Z. Li, B. Caswell, J. Ouyang, and G. E. Karniadakis. "Active Learning of Constitutive Relation from Mesoscopic Dynamics for Macroscopic Modeling of Non-Newtonian Flows," *Journal of Computational Physics* (February 2018), Elsevier. doi:10.1016/j.jcp.2018.02.039.

March

Asadi, M., B. Sayahpour, P. Abbasi, A. T. Ngo, K. Karis, J. R. Jokisaari, C. Liu, B. Narayanan, M. Gerard, P. Yasaei, X. Hu, A. Mukherjee, K. C. Lau, R. S. Assary, F. Khalili-Araghi, R. F. Klie, L. A. Curtiss, and A. Salehi-Khojin. "A Lithium-Oxygen Gattery with a Long Cycle Life in an Air-Like Atmosphere," *Nature* (March 2018), Springer Nature. doi:10.1038/nature25984.

Avilés-Casco, A. V., C. DeTar, D. Du, A. El-Khadra, A. Kronfeld, J. Laiho, and R. S. Van de Water. "B → D*lv at Non-Zero Recoil," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817513003.

Bai, Z., N. H. Christ, and C. T. Sachrajda. "The K_L-K_S Mass Difference," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817513017.

Bassman, L., A. Krishnamoorthy, A. Nakano, R. K. Kalia, H. Kumazoe, M. Misawa, F. Shimojo, and P. Vashishta. "Picosecond Electronic and Structural Dynamics in Photo-Excited Monolayer $MoSe_2$," *MRS Advances* (March 2018), Cambridge University Press. doi:10.1557/adv.2018.259.

Berman, D., B. Narayanan, M. J. Cherukara, S. K. R. S. Sankaranarayanan, A. Erdemir, A. Zinovev, and A. V. Sumant. "Operando Tribochemical Formation of Onion-Like-Carbons Leads to Macroscale Lubricity," *Nature Communications* (March 2018), Springer Nature. doi:10.1038/s41467-018-03549-6.

Brower, R., N. Christ, C. DeTar, R. Edwards, and P. Mackenzie. "Lattice QCD Application Development within the US DOE Exascale Computing Project," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817509010.

Chen, M., L. Zheng, B. Santra, H.-Y. Ko, R. A. DiStasio Jr., M. L. Klein, R. Car, and X. Wu. "Hydroxide Diffuses Slower Than Hydronium in Water Because Its Solvated Structure Inhibits Correlated Proton Structure," *Nature Chemistry* (March 2018), Springer Nature. doi:10.1038/s41557-018-0010-2.

Dawson, W., and F. Gygi. "Equilibration and Analysis of First-Principles Molecular Dynamics Simulations of Water," *The Journal of Chemical Physics* (March 2018), AIP. doi:10.1063/1.5018116.

Detar, C., S. Gottlieb, R. Li, and W. D. Toussaint. "MILC Code Performance on High End CPU and GPU Supercomputer Clusters," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817502009.

Gao, S., M. T. Young, J. X. Qiu, H.-J. Yoon, J. B. Christian, P. A. Fearn, G. D. Tourassi, and A. Ramanthan. "Hierarchical Attention Networks for Information Extraction from Cancer Pathology Reports," *Journal of the American Medical Informatics Association* (March 2018), Oxford University Press. doi:10.1093/jamia/ocx131.

Gennari, M., M. Vorabbi, A. Calci, and P. Navrátil. "Microscopic Optical Potential Derived from *Ab Initio* Translationally Invariant Nonlocal One-Body Densities," *Physical Review C* (March 2018), APS. doi:10.1103/PhysRevC.97.034619.

Guenther, J. N., S. Borsányi, Z. Fodor, S. D. Katz, A. Pásztor, and C. Ratti. "Fluctuations of Conserved Charges from Imaginary Chemical Potential," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817507036.

Hamilton, S. P. , S. R. Slattery, and T. M. Evans. "Multigorup Monte Carlo on GPUs: Comparison of History- and Event-Based Algorithms," *Annals of Nuclear Energy* (March 2018), Elsevier. doi:10.1016/j.anucene.2017.11.032.

Hong, S., C. Sheng, A. Krishnamoorthy, P. Rajak, S. Tiwari, K. Nomura, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. "Chemical Vapor Deposition Synthesis of MoS2 Layers from the Direct Sulfidation of MoO_3 Surfaces Using Reactive Molecular Dynamics Simulations," *The Journal of Physical Chemistry C* (March 2018), ACS. doi:10.1021/acs.jpcc.7b12035.

Kinnison, J., N. Kremer-Herman, D. Thain, and W. Scheirer. "SHADO: Massively Scalable Hardware-Aware Distributed Hyperparameter Optimization," *2018 IEEE Winter Conference on Applications of Computer Vision* (March 2018), Lake Tahoe, NV, IEEE. doi:10.1109/WACV.2018.00086.

Kumar, S. A. Humphrey, W. Usher, S. Petruzza, B. Peterson, J. A. Schmidt, D. Harris, B. Isaac, J. Thornock, T. Harman, V. Pascucci, and M. Berzins. "Scalable Data Management of the Uintah Simulation Framework for Next-Generation Engineering Problems with Radiation," *Supercomputing Frontiers* (March 2018), Springer Nature. doi:10.1007/978-3-319-69953-0_13.

Lee, M., and R. D. Moser. "Extreme-Scale Motions in Turbulent Plane Couette Flows," *Journal of Fluid Mechanics* (March 2018), Cambridge University Press. doi:10.1017/jfm.2018.131.

Li, X., F. S. Curtis, T. Rose, C. Schober, Á. Vázquez-Mayagoitia, K. Reuter, H. Oberhofer, and N. Marom. "Genarris: Random Generation of Molecular Crystal Structures and Fast Screening with a Harris Approximation," *The Journal of Chemical Physics* (March 2018), AIP. doi:10.1063/1.5014038.

Liu, Y., J. A. Bailey, A. Bazavov, C. Bernard, C. M. Bouchard, C. DeTar, D. Du, A. X. El-Khadra, E. D. Freeland, E. Gámiz, Z. Gelzer, S. Gottlieb, U. M. Heller, A. S. Kronfeld, J. Laiho, P. B. Mackenzie, Y. Meurice, E. T. Neil, J. N. Simone, R. Sugar, D. Toussaint, R. S. Van de Water, and R. Zhou. "B_s → $K\ell v$ Form Factors with 2+1 Flavors," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817513008.

Lu, P., D. Min, F. DiMaio, K. Y. Wei, M. D. Vahey, S. E. Boyken, Z. Chen, J. A. Fallas, G. Ueda, W. Sheffler, V. K. Mulligan, W. Xu, J. U. Bowie, and D. Baker. "Accurate Computational Design of Multipass Transmembrane Proteins," *Science* (March 2018), AAAS. doi:10.1126/science.aaq1739.

Nakamura, Y., Y. Kuramashi, and S. Takeda. "Critical Endline of the Finite Temperature Phase Transition for 2+1 Flavor QCD away from the SU(3)-Flavor Symmetric Point," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817507008.

Nicolau, B. G., A. Petronico, K. Letchworth-Weaver, Y. Ghadar, R. T. Haasch, J. A. N. T. Soares, R. T. Rooney, M. K. Y. Chan, A. A. Gewirth, and R. G. Nuzzo. "Controlling Interfacial Properties of Lithium-Ion Battery Cathodes with Alkylphosphonate Self-Assembled Monolayers," *Advanced Materials Interfaces* (March 2018), John Wiley and Sons. doi:10.1002/admi.201701292.

Osborn, J. C., and X.-Y. Jin. "A Staggered Eigensolver Based on Sparse Matrix Bidiagonalization," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817509011.

Ovchinnikov, S., H. Park, D. E. Kim, F. DiMaio, and D. Baker. "Protein Structure Prediciton Using Rosetta in CASP12," *Proteins* (March 2018), John Wiley and Sons. doi:10.1002/prot.25390.

Park, H. S. Ovchinnikov, D. E. Kim, F. DiMaio, and D. Baker. "Protein Homology Model Refinement by Large-Scale Energy Optimization," *PNAS* (March 2018), National Academy of Sciences. doi:10.1073/pnas.1719115115.

Pásztor, A., P. Alba, R. Bellwied, S. Borsányi, Z. Fodor, J. N. Günther, S. Katz, C. Ratti, V. M. Sarti, J. Noronha-Hostler, P. Parotto, I. P. Vazquez, V. Vovchenko, and H. Stoecker. "Hadron Thermodynamics from Imaginary Chemical Potentials," *35th International Symposium on Lattice Field Theory* (March 2018), EPJ Web of Conferences, EDP Sciences. doi:10.1051/epjconf/201817507046.

Ponga, M., and D. Sun. "A Unified Framework for Heat and Mass Transport at the Atomic Scale," *Modelling and Simulation in Materials Science and Engineering* (March 2018), IOP Publishing. doi:10.1088/1361-651x/aaaf94.

Poon, B. K., A. S. Brewster, and N. K. Sauter. "Deploying cctbx.xfel in Cloud Computing and High Performance Computing Environments," *Computational Crystallography Newsletter* (March 2018), Computational Crystallography.

Quaglioni, S., C. Romero-Redondo, P. Navrátil, and G. Hupin. "Three-Cluster Dynamics within the *Ab Initio* No-Core Shell Model with Continuum: How Many-Body Correlations and α Clustering Shape ^{6}He," *Physical Review C* (March 2018), APS. doi:10.1103/PhysRevC.97.034332.

Raimondi, F., G. Hupin, P. Navrátil, and S. Quaglioni. "^{7}Li(d,p)^{8}Li Transfer Reaction in the NCSM/RGM Approach," *Journal of Physics: Conference Series* (March 2018), IOP Publishing. doi:10.1088/1742-6596/981/1/012006.

Reisner, A., L. N. Olson, and J. D. Moulton. "Scaling Structured Multigrid to 500K+ Cores through Coarse-Grid Redistribution," *SIAM Journal on Scientific Computing* (March 2018), SIAM. doi:10.1137/17m1146440.

Seo, S. A. Amer, P. Balaji, G. Bosilca, A. Brooks, P. Carns, A. Castello, D. Genet, T. Herault, S. Iwasaki, P. Jindal, L. V. Kale, S. Krishnamoorthy, J. Lifflander, H. Lu, E. Meneses, M. Snir, Y. Sun, K. Taura, and P. Beckman. "Argobots: A Lightweight Low-Level Threading and Tasking Framework," *IEEE Transactions on Parallel and Distributed Systems* (March 2018), IEEE. doi:10.1109/tpds.2017.2766062.

Sobczyk, J. E., N. Rocco, A. Lovato, and J. Nieves. "Scaling within the Spectral Function Approach," *Physical Review C* (March 2018), APS. doi:10.1103/PhysRevC.97.035506.

Tan, J., T. Sinno, S. L. Diamond. "A Parallel Fluid Solid Coupling Model Using LAMMPS and Palabos Based on the Immersed Boundary Method," *Journal of Computational Science* (March 2018), Elsevier. doi:10.1016/j.jocs.2018.02.006.

Vorabbi, M., A. Calci, P. Navrátil, M. K. G. Kruse, S. Quaglioni, and G. Hupin. "Structure of the Exotic 9He Nucleus from the No-Core Shell Model with Continuum," *Physical Review C* (March 2018), APS. doi:10.1103/PhysRevC.97.034314.

Xie, S., L. Tu, Y. Han, L. Huang, K. Kang, K. U. Lao, P. Poddar, C. Park, D. A. Muller, R. A. DiStasio Jr., and J. Park. "Coherent, Atomically Thin Transition-Metal Dichalcogenide Superlattices with Engineered Strain," *Science* (March 2018), AAAS. doi:10.1126/science.aao5360.

April

Boughezal, R., A. Isgrò, and F. Petriello. "Next-to-Leading-Logarithmic Power Corrections for N-jettiness Subtraction in Color-Singlet Production," *Physical Review D* (April 2018), APS. doi:10.1103/PhysRevD.97.076006.

Curtis, F., T. Rose, and N. Marom. "Evolutionary Niching in the GAtor Genetic Algorithm for Molecular Crystal Structure Prediction," *Faraday Discussions* (April 2018), Royal Society of Chemistry. doi:10.1039/C8FD00067K.

Fang, J., J. J. Cambareri, C. S. Brown, J. Feng, A. Gouws, M. Li, and I. A. Bolotnov. "Direct Numerical Simulation of Reactor Two-Phase Flows Enabled by High-Performance Computing," *Nuclear Engineering and Design* (April 2018), Elsevier. doi:10.1016/j.nucengdes.2018.02.024.

Fodor, Z., K. Holland, J. Kuti, D. Nógrádi, and C. H. Wong. "Extended Investigation of the Twelve-Flavor β-Function," *Physics Letters B* (April 2018), Elsevier. doi:10.1016/j.physletb.2018.02.008.

Honga, K., S. Kurata, A. Jomphoak, M. Inada, K. Hayashi, and R. Maezono. "Stabilization Mechanism of the Tetragonal Structure in a Hydrothermally Synthesized BaTiO3 Nanocrystal," *Inorganic Chemistry* (April 2018), ACS. doi:10.1021/acs.inorgchem.8b00381.

Kim, J., A. D. Baczewski, T. D. Beaudet, A. Benali, M. Chandler Bennett, M. A. Berrill, N. S. Blunt, E. J. L. Borda, M. Casula, D. M. Ceperley, S. Chiesa, B. K. Clark, R. C. Clay III, K. T. Delaney, M. Dewing, K. P. Esler, H. Hao, O. Heinonen, P. R. C. Kent, J. T. Krogel, I. Kylänpää, Y. W. Li, M. G. Lopez, Y. Luo, F. D. Malone, R. M. Martin, A. Mathuriya, Jeremy, McMinis, C. A. Melton, L. Mitas, M. A. Morales, E. Neuscamman, W. D. Parker, S. D. P. Flores, N. A. Romero, B. M. Rubenstein, J. A. R. Shea, H. Shin, L. Shulenburger, A. F. Tillack, J. P. Townsend, N. M. Tubman, B. Van Der Goetz, J. E. Vincent, D. C. M. Yang, Y. Yang, S. Zhang, and L. Zhao. "QMCPACK: An Open Source *Ab Initio* Quantum Monte Carlo Package for the Electronic Structure of

Atoms, Molecules and Solids," *Journal of Physics: Condensed Matter* (April 2018), IOP Publishing. doi:10.1088/1361-648X/aab9c3.

König, S., and D. Lee. "Volume Dependence of N-Body Bound States," *Physical Letters B* (April 2018), Elsevier. doi:10.1016/j.physletb.2018.01.060.

Li, H., J. Yang, T. T. Chu, R. Naidu, L. Lu, R. Chandramohanadas, M. Dao, and G. E. Karniadakis. "Cytoskeleton Remodeling Induces Membrane Stiffness and Stability Changes of Maturing Reticulocytes," *Biophysical Journal* (April 2018), Elsevier. doi:10.1016/j.bpj.2018.03.004.

Moiz, A. A., P. Pal, D. Probst, Y. Pei, Y. Zhang, S. Som, and J. Kodavasal. "A Machine Learning-Genetic Algorithm (ML-GA) Approach for Rapid Optimization Using High-Performance Computing," *SAE International Journal of Commercial Vehicles* (April 2018), SAE International. doi:10.4271/2018-01-0190.

Morris, T. D., J. Simonis, S. R. Stroberg, C. Stumpf, G. Hagen, J. D. Holt, G. R. Jansen, T. Papenbrock, R. Roth, and A. Schwenk. "Structure of the Lightest Tin Isotopes," *Physical Review Letters* (April 2018), APS. doi:10.1103/PhysRevLett.120.152503.

Pan, K.-C., M. Liebendörfer, S. M. Couch, and F.-K. Thielemann. "Equation of State Dependent Dynamics and Multi-Messenger Signals from Stellar-Mass Black Hole Formation," *The Astrophysical Journal* (April 2018), IOP Publishing. doi:10.3847/1538-4357/aab71d.

Radice, D., E. Abdikamalov, C. D. Ott, P. Mösta, S. M. Couch, and L. F. Roberts. "Turbulence in Core-Collapse Supernovae," *Journal of Physics G: Nuclear and Particle Physics* (April 2018), IOP Publishing. doi:10.1088/1361-6471/aab872.

Regnier, D., N. Dubray, M. Verrière, and N. Schunck. "FELIX-2.0: New Version of the Finite Element Solver for the Time-Dependent Generator Coordinate Method with the Gaussian Overlap Approximation," *Computer Physics Communications* (April 2018), Elsevier. doi:10.1016/j.cpc.2017.12.007.

Scherbela, M., L. Hörmann, A. Jeindl, V. Obersteiner, and O. T. Hofmann. "Charting the Energy Landscape of Metal/Organic Interfaces via Machine Learning," *Physical Review Materials* (April 2018), APS. doi:10.1103/PhysRevMaterials.2.043803.

Shah, M. S., E. O. Fetisov, M. Tsapatsis, and J. I. Siepmann. "C2 Adsorption in Zeolites: In Silico Screening and Sensitivity to Molecular Models," *Molecular Systems Design and Engineering* (April 2018), Royal Society of Chemistry. doi:10.1039/C8ME00004B.

Song, S., M.-C. Kim, E. Sim, A. Benali, O. Heinonen, and K. Burke. "Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes," *Journal of Chemical Theory and Computation* (April 2018), ACS. doi:10.1021/acs.jctc.7b01196.

Tran, D. T., H. J. Ong, G. Hagen, T. D. Morris, N. Aoi, T. Suzuki, Y. Kanada-En'yo, L. S. Geng, S. Terashima, I. Tanihata, T. T. Nguyen, Y. Ayyad, P. Y. Chan, M. Fukuda, H. Geissel, M. N. Harakeh, T. Hashimoto, T. H. Hoang, E. Ideguchi, A. Inoue, G. R. Jansen, R. Kanungo, T. Kawabata, L. H. Khiem, W. P. Lin, K. Matsuta, M. Mihara, S. Momota, D. Nagae, N. D. Nguyen, D. Nishimura, T. Otsuka, A. Ozawa, P. P. Ren, H. Sakaguchi, C. Scheidenberger, J. Tanaka, M. Takechi, R. Wada, and T. Yamamoto. "Evidence for Prevalent Z=6 Magic Number in Neutron-Rich Carbon Isotopes," *Nature Communications* (April 2018), Springer Nature. doi:10.1038/s41467-018-04024-y.

May

Alexeev, Y. "Evaluation of the Intel-QS Performance on Theta Supercomputer," *Argonne Leadership Computing Facility* (May 2018), Lemont, IL, Argonne National Laboratory.

Bak, S., H. Menon, S. White, M. Diener, and L. Kale. "Multi-Level Load Balancing with an Integrated Runtime Approach," *2018 18th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing* (May 2018), Washington, D.C., IEEE. doi:10.1109/CCGRID.2018.00018.

Bourouaine, S., and J. C. Perez. "On the Limitations of Taylor's Hypothesis in Parker Solar Probe's Measurements near the Alfvén Critical Point," *The Astrophysical Journal Letters* (May 2018), IOP Publishing. doi:10.3847/2041-8213/aabccf.

Child, H. L., S. Habib, K. Heitmann, N. Frontiere, H. Finkel, A. Pope, and V. Morozov. "Halo Profiles and the Concentration-Mass Relation for a ΛCDM Universe," *The Astrophysical Journal* (May 2018), IOP Publishing. doi:10.3847/1538-4357/aabf95.

Chunduri, S., M. Ghaffari, M. S. Lahijani, A. Srinivasan, and S. Namilae. "Parallel Low Discrepancy Parameter Sweep for Public Health Policy," *2018 18th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing* (May 2018), Washington, D.C., IEEE. doi:10.29007/vp3d.

Gaiduk, A. P., J. Gustafson, F. Gygi, and G. Galli. "First-Principles Simulations of Liquid Water Using a Dielectric-Dependent Hybrid Functional," *The Journal of Physical Chemistry Letters* (May 2018), ACS. doi:10.1021/acs.jpclett.8b01017.

Kettimuthu, R., Z. Liu, D. Wheeler, I. Foster, K. Heitmann, and F. Cappello. "Transferring a Petabyte in a Day," *Future Generation Computer Systems* (May 2018), Elsevier. doi:10.1016/j.future.2018.05.051.

Kuriki, R., T. Ichibha, K. Hongo, D. Lu, R. Maezono, H. Kageyama, O. Ishitani, K. Oka, and K. Maeda. A Stable, Narrow-Gap Oxyfluoride Photocatalyst for Visible-Light Hydrogen Evolution and Carbon Dioxide Reduction," *Journal of the American Chemical Society* (May 2018), ACS. doi:10.1021/jacs.8b02822.

Liu, J., E. Tennessen, J. Miao, Y. Huang, J. M. Rondinelli, and H. Heinz. Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations," *The Journal of Physical Chemistry C* (May 2018), ACS. doi:10.1021/acs.jpcc.8b01891.

Oshima, T., T. Ichibha, K. S. Qin, K. Muraoka, J. J. M. Vequizo, K. Hibino, R. Kuriki, S. Yamashita, K. Hongo, T. Uchiyama, K. Fujii, D. Lu, R. Maezono, A. Yamakata, H Kato, K. Kimoto, M. Yashima, Y. Uchimoto, M. Kakihana, O. Ishitani, H. Kageyama, and K. Maeda. "Undoped Layered Perovskite Oxynitride $Li_2LaTa_2O_6N$ for Photocatalytic CO_2 Reduction with Visible Light," *Angewandte Chemie* (May 2018), Wiley-VCH. doi:10.1002/anie.201803931.

Petersen, M., X. Asay-Davis, A. Berres, Q. Chen, N. Feige, D. Jacobsen, P. Jones, M. Maltrud, T. Ringler, G. Streletz, A. Turner, L. Van Roekel, M. Veneziani, J. Wolfe, P. Wolfram, and J. Woodring. "An Evaluation of the Ocean and Sea Ice Climate of E3SM Using MPAS and Interannual CORE-II Forcing," *Journal of Advances in Modeling Earth Systems* (May 2018), Wiley and Sons. doi:10.5281/zenodo.1246339.

Pryor Jr., A., A. Rana, R. Xu, J. A. Rodriguez, Y. Yang, M. Gallagher-Jones, H. Jiang, K. Kanhaiya, M. Nathanson, J. Park, S. Kim, S. Kim, D. Nam, Y. Yue, J. Fan, Z. Sun, B. Zhang, D. F. Gardner, C. S. B. Dias, Y. Joti, T. Hatsui, T. Kameshima, Y. Inubushi, K. Tono, J. Y. Lee, M. Yabashi, C. Song, T. Ishikawa, H. C. Kapteyn, M. M. Murnane, H. Heinz, and J. Miao. "Single-Shot 3D Coherent Diffractive Imaging of Core-Shell Nanoparticles with Elemental Specificity," *Scientific Reports* (May 2018), Springer Nature. doi:10.1038/s41598-018-26182-1.

Rocco, N., W. Leidemann, A. Lovato, and G. Orlandini. "Relativistic Effects in *Ab Initio* Electron-Nucleus Scattering," *Physical Review C* (May 2018), APS. doi:10.1103/PhysRevC.97.055501.

Shi, Y., B. Song, R. Shahbazian-Yassar, J. Zhao and W. A. Saidi. "Experimentally Validated Structures of Supported Metal Nanoclusters on MoS_2," *The Journal of Physical Chemistry Letters* (May 2018), ACS. doi:10.1021/acs.jpclett.8b01233.

Srihakulung, S., R. Maezono, P. Toochinda, W. Kongprawechnon, A. Intarapanich, and L. Lawtrakul. "Host-Guest Interactions of Plumbagin with β-Cyclodextrin, Dimethyl-β-Cyclodextrin and Hydroxypropyl-β-Cyclodextrin: Semi-Empirical Quantum Mechanical PM6 and PM7 Methods," *Scientia Pharmaceutica* (May 2018), MDPI. doi:10.3390/scipharm86020020.

Steinbrecher, P., H.-T. Ding, F. Karsch, S. Mukherjee, and H. Ohno. "QCD Transition at Zero and Non-Zero Baryon Densities," *The 27th International Conference on Ultrarelativistic Nucleus-Nucleus Collisions* (May 2018), Lido di Venezia, CERN.

Tang, H., S. Byna, F. Tessier, T. Wang, B. Dong, J. Mu, Q. Koziol, J. Soumagne, V. Vishwanath, J. Liu, and R. Warren. "Toward Scalable and Asynchronous Object-Centric Data Management for HPC," *2018 18th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing* (May 2018), Washington, D.C., IEEE. doi:10.1109/CCGRID.2018.00026.

Wang, X., X. Liu, C. Cook, B. Schatschneider, and N. Marom. "On the Possibility of Singlet Fission in Crystalline Quaterrylene," *The Journal of Chemical Physics* (May 2018), AIP. doi:10.1063/1.5027553.

Wang, Y., H. Guo, Q. Zheng, W. A. Saidi, and J. Zhao. "Tuning Solvated Electrons by Polar-Nonpolar Oxide Heterostructure," *The Journal of Physical Chemistry Letters* (May 2018), ACS. doi:10.1021/acs.jpclett.8b00938.

William, T. J. "Early Science on Theta," *Computing in Science and Engineering* (May 2018), AIP. doi:10.1109/mcse.2018.03202630.

Yang, F., and A. A. Chien. "Large-Scale and Extreme-Scale Computing with Stranded Green Power: Opportunities and Costs," *IEEE Transactions on Parallel and Distributed Systems* (May 2018), IEEE. doi:10.1109/tpds.2017.2782677.

Zhao, D., and H. Aluie. "Inviscid Criterion for Decomposing Scales," *Physical Review Fluids* (May 2018), APS. doi:10.1103/PhysRevFluids.3.054603.

Zheng, H., H. J. Changlani, K. T. Williams, B. Busemeyer, and L. K. Wanger. "From Real Materials to Model Hamiltonians With Density Matrix Downfolding," *Frontiers in Physics* (May 2018), Frontiers Media. doi:10.3389/fphy.2018.00043.

Zheng, Q., Y. Xie, Z. Lan, O. V. Prezhdo, W. A. Saidi, and J. Zhao. "Phonon-Coupled Ultrafast Interlayer Charge Oscillation at van der Waals Heterostructure Interfaces," *Physical Review B* (May 2018), APS. doi:10.1103/PhysRevB.97.205417.

Zou, L. W. A. Saidi, Y. Lei, Z. Liu, J. Li, L. Li, Q. Zhu, D. Zakharov, E. A. Stach, J. C. Yang, G. Wang, and G. Zhou. "Segregation Induced Order-Disorder Transition in Cu(Au) Surface Alloys," *Acta Materialia* (May 2018), Elsevier. doi:10.1016/j.actamat.2018.05.040.

June

Benali, A., Y. Luo, H. Shin, D. Pahls, and O. Heinonen. "Quantum Monte Carlo Calculations of Catalytic Energy Barriers in a Metallorganic Framework with Transition-Metal-Functionalized Nodes," *The Journal of Physical Chemistry C* (June 2018), ACS. doi:10.1021/acs.jpcc.8b02368.

Chard, R., R. Vescovi, M. Du, H. Li, K. Chard, S. Tuecke, N. Kasthuri, and I. Foster. "High-Throughput Neuroanatomy and Trigger-Action Programming: A Case Study in Research Automation," *Proceedings of the 1st International Workshop on Autonomous Infrastructure for Science* (June 2018), New York, NY, ACM. doi:10.1145/3217197.3217206.

DeJaco, R. F., B. Elyassi, M. D. de Mello, N. Mittal, M. Tsapatsis, and J. I. Siepmann. "Understanding the Unique Sorption of Alkane- α, ω-Diols in Silicalite-1," *The Journal of Chemical Physics* (June 2018). doi:10.1063/1.5026937.

Guo, H., C. Zhao, Q. Zheng, Z. Lan, O. V. Prezhdo, W. A. Saidi, and J. Zhao. "Superatom Molecular Orbital as an Interfacial Charge Separation State," *The Journal of Physical Chemistry Letters* (June 2018), ACS. doi:10.1021/acs.jpclett.8b01302.

Houston, M. L., J. W. Nichols, F. Zigunov, P. Sellappan, and F. S. Alvi. "Simulations and Experiments of Dual High-Speed Impinging Jets," *2018 AIAA/CEAS Aeroacoustics Conference* (June 2018), Atlanta, GA, AIAA. doi:10.2514/6.2018-2825.

Jeun, J., and J. W. Nichols. "Non-Compact Sources of Sound in High-Speed Turbulent Jets Using Input-Output Analysis," *2018 AIAA/CEAS Aeroacoustics Conference* (June 2018), Atlanta, GA, AIAA. doi:10.2514/6.2018-3467.

Nalewajko, K., Y. Yuan, and M. Chruślińska. "Kinetic Simulations of Relativistic Magnetic Reconnection with Synchrotron and Inverse Compton Cooling," *Journal of Plasma Physics* (June 2018), Cambridge University Press. doi:10.1017/S0022377818000624.

Planas, J., F. Delalondre, and F. Schürmann. "Accelerating Data Analysis in Simulation Neuroscience with Big Data Technologies," *International Conference on Computational Science* (June 2018), Springer Nature. doi:10.1007/978-3-319-93698-7_28.

Poggie, J., and K. M. Porter. "Numerical Simulation of Sidewall Influence on Supersonic Compression Ramp Interactions," *2018 Fluid Dynamics Conference* (June 2018), Atlanta, GA, AIAA. doi:10.2514/6.2018-4029.

Rada, B. K., D. Suh, and B. Roux. "A Generalized Linear Response Framework for Expanded Ensemble and Replica Exchange Simulations," *The Journal of Chemical Physics* (June 2018), AIP. doi:10.1063/1.5027494.

Ruyer, C., and F. Fiuza. "Disruption of Current Filaments and Isotropization of the Magnetic Field in Counterstreaming Plasmas," *Physical Review Letters* (June 2018), APS. doi:10.1103/PhysRevLett.120.245002.

Schanen, M., F. Gilbert, C. G. Petra, and M. Anitescu. "Toward Multiperiod AC-Based Contingency Constrained Optimal Power Flow at Large Scale," *2018 Power Systems Computation Conference* (June 2018), Dublin, Ireland, IEEE. doi:10.23919/PSCC.2018.8442590.

Tessier, F., P. Gressier, and V. Vishwanath. "Optimizing Data Aggregation by Leveraging the Deep Memory Hierarchy on Large-Scale Systems." *Proceedings of the 2018 International Conference on Supercomputing* (June 2018), Beijing, China, ACM. doi:10.1145/3205289.3205316.

Xu, L., R. Gordon, R. Farmer, A. Pattanayak, A. Binkowski, X. Huang, M. Avram, A. Krishna, E. Voll, J. Pavesse, J. Chavez, J. Bruce, A. Mazar, A. Nibbs, W. Anderson, L. Li, B. Jovanovic, S. Pruell, M. Valsecchi, G. Francia, R. Betori, K. Scheidt, and R. Bergan. "Precision Therapeutic Targeting of Human Cancer Cell Motility," *Nature Communications* (June 2018), Springer Nature. doi:10.1038/s41467-018-04465-5.

Zarrouk, P., E. Burtin, H. Gil-Marín, A. J. Ross, R. Tojeiro, I. Pâris, K. S. Dawson, A. D. Myers, W. J. Percival, C.-H. Chuang, G.-B. Zhao, J. Bautista, J. Comparat, V. González-Pérez, S. Habib, K. Heitmann, J. Hou, P. Laurent, J.-M. Le Goff, F. Prada, S. A. Rodríguez-Torres, G. Rossi, R. Ruggeri, A. G. Sánchez, D. P. Schneider, J. L. Tinker, Y. Wang, C. Yèche, F. Baumgarten, J. R. Brownstein, S. de la Torre, H. du Mas des Bourboux, J.-P. Kneib, V. Mariappan, N. Palanque-Delabrouille, J. Peacock, P. Petitjean, H.-J. Seo, and C. Zhao. "The Clustering of the SDSS-IV Extended Baryon Oscillation Spectroscopic Survey DR14 Quasar Sample: Measurement of the Growth Rate of Structure from the Anisotropic Correlation Function between Redshift 0.8 and 2.2," *Monthly Notices of the Royal Astronomical Society* (June 2018), Oxford University Press. doi:10.1093/mnras/sty506.

Zhai, K., T. Banerjee, D. Zwick, J. Hackl, and S. Ranka. "Dynamic Load Balancing for Compressible Multiphase Turbulence," *Proceedings of the 2018 International Conference on Supercomputing* (June 2018), Beijing, China, ACM. doi:10.1145/3205289.3205304.

July

Aguilar, M., et al. (AMS collaboration). "Observation of Fine Time Structures in the Cosmic Proton and Helium Fluxes with the Alpha Magnetic Spectrometer on the International Space Station," *Physical Review Letters* (July 2018), APS. doi:10.1103/PhysRevLett.121.051101.

Aguilar, M., et al. (AMS collaboration). "Precision Measurement of Cosmic-Ray Nitrogen and Its Primary and Secondary Components with the Alpha Magnetic Spectrometer on the International Space Station," *Physical Review Letters* (July 2018), APS. doi:10.1103/PhysRevLett.121.051103.

Asch, M., T. Moore, R. Badia, M. Beck, P. Beckman, T. Bidot, F. Bodin, F. Cappello, A. Choudhary, B. de Supinski, E. Deelman, J. Dongarra, A. Dubey, G. Fox, H. Fu, S. Girona, W. Gropp, M. Heroux, Y. Ishikawa, K. Keahey, D. Keyes, W. Kramer, J.-F. Lavignon, Y. Lu, S. Matsuoka, B. Mohr, D. Reed, S. Requena, J. Saltz, T. Schulthess, R. Stevens, M. Swany, A. Szalay, W. Tang, G. Varoquaux, J.-P. Vilotte, R. Wisniewski, Z. Xu, and I. Zacharov. "Big Data and Extreme-Scale Computing," *The International Journal of High Performance Computing Applications* (July 2018), SAGE Publications. doi:10.1177/1094342018778123.

Bassman, L., A. Krishnamoorthy, H. Kumazoe, M. Misawa, F. Shimojo, R. K. Kalia, A. Nakano, and P. Vashishta. "Electronic Origin of Optically-Induced Sub-Picosecond Lattice Dynamics in $MoSe_2$ Monolayer," *Nano Letters* (July 2018), ACS. doi:10.1021/acs.nanolett.8b00474.

Binder, S., A. Calci, E. Epelbaum, R. J. Furnstahl, J. Golak, K. Hebeler, T. Hüther, H. Kamada, H. Krebs, P. Maris, U.-G. Meißner, A. Nogga, R. Roth, R. Skibiński, K. Topolnicki, J. P. Vary, K. Vobig, and H. Witała. "Few-Nucleon and Many-Nucleon Systems with Semilocal Coordinate-Space Regularized Chiral Nucleon-Nucleon Forces," *Physical Review C* (July 2018), APS. doi:10.1103/PhysRevC.98.014002.

Blum, T., P. A. Boyle, V. Gülpers, T. Izubuchi, L. Jin, C. Jung, A. Jüttner, C. Lehner, A. Portelli, and J. T. Tsang. "Calculation of the Hadronic Vacuum Polarization Contribution to the Muon Anomalous Magnetic Moment," *Physical Review Letters* (July 2018), APS. doi:10.1103/PhysRevLett.121.022003.

Borsányi, S., Z. Fodor, M. Giordano, S. D. Katz, A. Pásztor, C. Ratti, A. Schäfer, K. K. Szabó, and B. C. Tóth. "High Statistics Lattice Study of Stress Tensor Correlators in Pure SU(3) Gauge Theory," *Physical Review D* (July 2018), APS. doi:10.1103/PhysRevD.98.014512.

Cruz-León, S., Á. Vázquez-Mayagoitia, S. Melchionna, N. Schwierz, and M. Fyta. "Coarse-Grained Double-Stranded RNA Model from Quantum-Mechanical Calculations," *They Journal of Physical Chemistry B* (July 2018), ACS. doi:10.1021/acs.jpcb.8b03566.

Frame, D., R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj. "Eigenvector Continuation with Subspace Learning," *Physical Review Letters* (July 2018), APS. doi:10.1103/PhysRevLett.121.032501.

Hou, J., A. G. Sánchez, R. Scoccimarro, S. Salazar-Albornoz, E. Burtin, H. Gil-Marín, W. J. Percival, R. Ruggeri, P. Zarrouk, G.-B. Zhao, J. Bautista, J. Brinkmann, J. R. Brownstein, K. S. Dawson, N. C. Devi, A. D. Myers, S. Habib, K. Heitmann, R. Tojeiro, G. Rossi, D. P. Schneider, H.-J. Seo, and Y. Wang. "The Clustering of the SDSS-IV Extended Baryon Oscillation Spectroscopic Survey DR14 Quasar Sample: Anisotropic Clustering Analysis in Configuration Space," *Monthly Notices of the Royal Astronomical Society* (July 2018), Oxford University Press. doi:10.1093/mnras/sty1984.

Jansen, K. E., M. Rasquin, J. A. Farnsworth, N. Rathay, M. C. Monastero, and M. Amitay. "Interaction of a Synthetic Jet with Separated Flow over a Vertical Tail," *AIAA Journal* (July 2018), AIAA. doi:10.2514/1.j056751.

Kim, K.-S., M. H. Han, C. Kim, Z. Li, G. E. Karniadakis, and E. K. Lee. "Nature of INstrinsic Uncertainties in Equilibrium Molecular Dynamics Estimation of Shear Viscosity for Simple and Complex Fluids," *The Journal of Chemical Physics* (July 2018), AIP. doi:10.1063/1.5035119.

Klein, N., S. Elhatisari, T. A. Lähde, D. Lee, and U.-G. Meißner. "The Tjon Band in Nuclear Lattice Effective Field Theory," *The European Physical Journal A* (July 2018), Springer Nature. doi:10.1140/epja/i2018-12553-y.

Kumazoe, H., A. Krishnamoorthy, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. "Photo-Induced Lattice Contraction in Layered Materials," *Journal of Physics: Condensed Matter* (July 2018), IOP Publishing. doi:10.1088/1361-648X/aad022.

Li, J., M. Bouchard, P. Reiss, D. Aldakov, S. Pouget, R. Demadrille, C. Aumaitre, B. Frick, D. Djurado, M. Rossi, and P. Rinke. "Activation Energy of Organic Cation Rotation in $CH_3NH_3PbI_3$ and $CD_3NH_3PbI_3$: Quasi-Elastic Neutron Scattering Measurements and First-Principles Analysis Including Nuclear Quantum Effects," *The Journal of Physical Chemistry Letters* (July 2018), ACS. doi:10.1021/acs.jpclett.8b01321.

Li, J., J. Järvi, and P. Rinke. "Multiscale Model for Disordered Hybrid Perovskites: The Concept of Organic Cation Pair Modes," *Physical Review B* (July 2018), APS. doi:10.1103/PhysRevB.98.045201.

Matri, P., P. Carns, R. Ross, A. Costan, M. S. Perez, and G. Antoniu. "SLoG: Large-Scale Logging Middleware for HPC and Big Data Convergence," *2018 IEEE 38th International Conference on Distributed Computing Systems* (July 2018), Vienna, Austria, IEEE. doi:10.1109/ICDCS.2018.00156

Peterson, B., A. Humphrey, J. Holmen, T. Harman, M. Berzins, D. Sunderland, and H. C. Edwards. "Demonstrating GPU Code Portability and Scalability for Radiative Heat Transfer Computations," *Journal of Computational Science* (July 2018), Elsevier. doi:10.1016/j.jocs.2018.06.005.

Ratti, C. "Lattice QCD and Heavy Ion Collisions: A Review of Recent Progress," *Reports on Progress in Physics* (July 2018), IOP Publishing. doi:10.1088/1361-6633/aabb97.

Shin, H., A. Benali, Y. Luo, E. Crabb, A. Lopez-Bezanilla, L. E. Ratcliff, A. M. Jokisaari, and O. Heinonen. "Zirconia and Hafnia Polymorphs: Ground-State Structural Properties from Diffusion Monte Carlo," *Physical Review Materials* (July 2018), APS. doi:10.1103/PhysRevMaterials.2.075001.

Song, B., K. He, Y. Yuan, S. Sharifi-Asi, M. Cheng, J. Lu, W. A. Saidi, and R. Shahbazian-Yassar. "In Situ Study of Nucleation and Growth Dynamics of Au Nanoparticles on MoS2 Nanoflakes," *Nanoscale* (July 2018), Royal Society of Chemistry. doi:10.1039/C8NR03519A.

Vincenti, H., and J.-L. Vay. "Ultrahigh-Order Maxwell Solver with Extreme Scalability for Electromagnetic PIC Simulations of Plasmas," *Computer Physics Communications* (July 2018), Elsevier. doi:10.1016/j.cpc.2018.03.018.

Yu, L., Z. Zhou, Y. Fan, M. E. Papka, and Z. Lan. "System-Wide Trade-Off of Performance, Power, and Resilience on Petascale Systems," *The Journal of Supercomputing* (July 2018), Springer Nature. doi:10.1007/s11227-018-2368-8.

August

Ahn, J., I. Hong, Y. Kwon, R. C. Clay, L. Shulenburger, H. Shin, and A. Benali. "Phase Stability and Interlayer Interaction of Blue Phosphorene," *Physical Review B* (August 2018), APS. doi:10.1103/PhysRevB.98.085429.

Allcock, W., B. Bernardoni, C. Bertoni, N. Getty, J. Insley, M. E. Papka, S. Rizzi, and B. Toonen. "RAM as a Network Managed Resource," *2018 IEEE International Parallel and Distributed Processing Symposium Workshops* (August 2018), Vancouver, Canada, IEEE. doi:10.1109/ipdpsw.2018.00024.

Di, S., H. Guo, R. Gupta, E. R. Pershey, M. Snir, and F. Cappello. "Exploring Properties and Correlations of Fatal Events in a Large-Scale HPC System," *IEEE Transactions on Parallel and Distributed Systems* (August 2018), IEEE. doi:10.1109/TPDS.2018.2864184.

Fairbanks, H. R., L. Jofre, G. Geraci, G. Iaccarino, and A. Doostan. "Bi-fidelity Approximation For Uncertainty Quantification And Sensitivity Analysis Of Irradiated Particle-Laden Turbulence," *Office of Scientific and Technical Information* (August 2018), U.S. Department of Energy. doi:10.2172/1463950.

Fang, J., J. J. Cambareri, M. Rasquin, A. Gouws, R. Balakrishnan, K. E. Jansen, and I. A. Bolotnov. "Interface Tracking Investigation of Geometric Effects on the Bubbly Flow in PWR Subchannels," *Nuclear Science and Engineering* (August 2018), American Nuclear Society. doi:10.1080/00295639.2018.1499280.

Fetisov, E. O., M. S. Shah, J. R. Long, M. Tsapatsis, and J. I. Siepmann. "First Principles Monte Carlo Simulations of Unary and Binary Adsorption: CO_2, N_2, and H_2O in Mg-MOF-74," *Chemical Communications* (August 2018), Royal Society of Chemistry. doi:10.1039/C8CC06178E.

Freer, M., H. Horiuchi, Y. Kanada-En'yo, D. Lee, and U.-G. Meißner. "Microscopic Clustering in Light Nuclei," *Reviews of Modern Physics* (August 2018), APS. doi:10.1103/RevModPhys.90.035004.

Hunt, R. J., M. Szyniszewski, G. I. Prayogo, R. Maezono, and N. D. Drummond. "Quantum Monte Carlo Calculations of Energy Gaps from First Principles," *Physical Review B* (August 2018), APS. doi:10.1103/PhysRevB.98.075122.

Li, H., D. P. Papageorgiou, H.-Y. Chang, L. Lu, J. Yang, and Y. Deng. "Synergistic Integration of Laboratory and Numerical Approaches in Studies of the Biomechanics of Diseased Red Blood Cells," *Biosensors* (August 2018), MDPI. doi:10.3390/bios8030076.

Lu, L., Y. Deng, X. Li, H. Li, and G. E. Karniadakis. "Understanding the Twisted Structure of Amyloid Fibrils via Molecular Simulations," *The Journal of Physical Chemistry B* (August 2018), ACS. doi:10.1021/acs.jpcb.8b07255.

Luo, Y., K. P. Esler, P. R. C. Kent, and L. Shulenburger. "An Efficient Hybrid Orbital Representation for Quantum Monte Carlo Calculations," *The Journal of Chemical Physics* (August 2018), AIP. doi:10.1063/1.5037094.

Marrinan, T., S. Rizzi, J. Insley, B. Toonen, W. Allcock, and M. E. Papka. "Transferring Data from High-Performance Simulations to Extreme Scale Analysis Applications in Real-Time," *2018 IEEE International Parallel and Distributed Processing Symposium Workshops* (August 2018), Vancouver, Canada, IEEE. doi:10.1109/IPDPSW.2018.00188.

Mishra, A., S. Hong, C. Sheng, K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta. "Multiobjective Genetic Training and Uncertainty Quantification of Reactive Force Fields," *npj Computational Materials* (August 2018), Springer Nature. doi:10.1038/s41524-018-0098-3.

Pan, D., M. Govoni, and G. Galli. "Communication: Dielectric Properties of Condensed Systems Composed of Fragments," *The Journal of Chemical Physics* (August 2018), AIP. doi:10.1063/1.5044636.

Patra, T. K., D. S. Schulman, H. Chan, M. J. Cherukara, M. Terrones, S. Das, B. Narayanan, and S. K. R. S. Sankaranarayanan. "Defect Dynamics in 2-D MoS_2 Probed by Using Machine Learning, Atomistic Simulations, and High-Resolution Microscopy," *ACS Nano* (August 2018), ACS. doi:10.1021/acsnano.8b02844.

Rajak, P., R. K. Kalia, A. Nakano, and P. Vashishta. "Faceting, Grain Growth, and Crack Healing in Alumina," *ACS Nano* (August 2018), ACS. doi:10.1021/acsnano.8b02484.

Restrepo, D. and R. Taborda. "Multiaxial Cyclic Plasticity in Accordance with 1D Hyperbolic Models and Masing Criteria," *International Journal for Numerical and Analytical Methods in Geomechanics* (August 2018), John Wiley and Sons. doi:10.1002/nag.2845.

Setyawan, W., M. W. D. Cooper, K. J. Roche, R. J. Kurtz, B. P. Uberuaga, D. A. Andersson, and B. D. Wirth. "Atomistic Model of Xenon Gas Bubble Re-Solution Rate Due to Thermal Spike in Uranium Oxide," *Journal of Applied Physics* (August 2018), AIP. doi:10.1063/1.5042770.

Tondravi, M., W. Scullin, M. Du, R. Vescovi, V. De Andrade, C. Jacobsen, K. P. Kording, D. Gürsoy, and E. Dyer. "A Pipeline for Distributed Segmentation of Teravoxel Tomography Datasets," *Microscopy and Microanalysis* (August 2018), Cambridge University Press. doi:10.1017/s143192761801320x.

Various. "Active Flow and Combustion Control 2018," *Active Flow and Combustion Control* (August 2018), Berlin, Germany, Springer Nature. doi:10.1007/978-3-319-98177-2.

Wang, X., M. Mubarak, X. Yang, R. B. Ross, and Z. Lan. "Trade-Off Study of Localizing Communication and Balancing Network Traffic on a Dragonfly System," *2018 IEEE International Parallel and Distributed Processing Symposium* (August 2018), Vancouver, Canada, IEEE. doi:10.1109/IPDPS.2018.00120.

Willa, R., A. E. Koshelev, I. A. Sadovskyy, and A. Glatz. "Peak Effect Due to Competing Vortex Ground States in Superconductors with Large Inclusions," *Physical Review B* (Agust 2018), APS. doi:10.1103/PhysRevB.98.054517.

Zhang, H., R. T. Mills, K. Rupp, and B. F. Smith. "Vectorized Parallel Sparse Matrix-Vector Multiplication in PETSc Using AVX-512," *Proceedings of the 47th International Conference on Parallel Processing* (August 2018), Eugene, OR, ACM. doi:10.1145/3225058.3225100.

September

Bazavov, A., C. Bernard, N. Brambilla, N. Brown, C. DeTar, A.X. El-Khadra, E. Gámiz, Steven Gottlieb, U.M. Heller, J. Komijani, A.S. Kronfeld, J. Laiho, P.B. Mackenzie, E. T. Neil, J.N. Simone, R.L. Sugar, D. Toussaint, A. Vairo, and R.S. Van de Water. "Up-, Down-, Strange-, Charm-, and Bottom-Quark Masses from Four-Flavor Lattice QCD," *Physical Review D* (September 2018), APS. doi:10.1103/PhysRevD.98.054517.

Boughezal, R., F. Petriello, and H. Xing. "Inclusive Jet Production as a Probe of Polarized Parton Distribution Functions at a Future EIC," *Physical Review D* (September 2018), APS. doi:10.1103/PhysRevD.98.054031.

Cherukara, M. J., R. Rokharel, T. S. O'Leary, J. K. Baldwin, E. Maxey, W. Cha, J. Maser, R. J. Harder, S. J. Fensin, and R. L. Sandberg. "Three-Dimensional X-ray Diffraction Imaging of Dislocations in Polycrystalline Metals under Tensile Loading," *Nature Communications* (September 2018), Springer Nature. doi:10.1038/s41467-018-06166-5.

Gharaei, S. K., M. Abbasnejad, and R. Maezono. "Bandgap Reduction of Photocatalytic TiO_2 Nanotube by Cu Doping," *Scientific Reports* (September 2018), Springer Nature. doi:10.1038/s41598-018-32130-w.

Guenther, J. N. S. Borsanyi, Z. Fodor, S. K. Katz, K. K. Szabó, A. Pasztor, I. Portillo, and C. Ratti. "Lattice Thermodynamics at Finite Chemical Potential from Analytical Continuation," *Journal of Physics: Conference Series* (September 2018), IOP Publishing. doi:10.1088/1742-6596/1070/1/012002.

Jiang, Y.-F., M. Cantiello, L. Bildsten, E. Quataert, O. Blaes, and J. Stone. "Outbursts of Luminous Blue Variable Stars from Variations in the Helium Opacity," *Nature* (September 2018), Springer Nature. doi:10.1038/s41586-018-0525-0.

Li, H., L. Lu, X. Li, P. A. Buffet, M. Dao, G. E. Karniadakis, and S. Suresh. "Mechanics of Diseased Red Blood Cells in Human Spleen and Consequences for Hereditary Blood Disorders," *PNAS* (September 2018), National Academy of Sciences. doi:10.1073/pnas.1806501115.

Marjanovic, G., J. Hackl, M. Shringarpure, S. Annamalai, T. L. Jackson, and S. Balachandar. "Inviscid Simulations of Expansion Waves Propagating into Structured Particle Beds at Low Volume Fractions," *Physical Review Fluids* (September 2018), APS. doi:10.1103/PhysRevFluids.3.094301.

O'Connor, E., R. Bollig, A. Burrows, S. Couch, T. Fischer, H.-T. Janka, K. Kotake, E. J. Lentz, M. Liebendörfer, O. E. Bronson Messer, A. Mezzacappa, T. Takwaki, and D. Vartanyan. "Global Comparison of Core-Collapse Supernova Simulations in Spherical Symmetry," *Journal of Physics G: Nuclear and Particle Physics* (September 2018), IOP Publishing. doi:10.1088/1361-6471/aadeae.

O'Connor, E., and S. M. Couch. "Exploring Fundamentally Three-Dimensional Phenomena in High-Fidelity Simulations of Core-Collapse Supernovae," *The Astrophysical Journal* (September 2018), IOP Publishing. doi:10.3847/1538-4357/aadcf7.

Papageorgiu, D. P., S. Z. Abidi, H.-Y. Chang, X. Li, G. J. Kato, G. E. Karniadakis, S. Suresh, and M. Dao. "Simultaneous Polymerization and Adhesion under Hypoxia in Sickle Cell Disease," *PNAS* (August 2018), National Academy of Sciences. doi:10.1073/pnas.1807405115.

Pramanik, C., D. Nepal, M. Nathanson, J. R. Gissinger, A. Garley, R. J. Berry, A. Davijani, S. Kumar, and H. Heinz. "Molecular Engineering of Interphases in Polymer/Carbon Nanotube Composites to Reach the Limits of Mechanical Performance," *Composites Science and Technology* (September 2018), Elsevier. doi:10.1016/j.compscitech.2018.04.013.

Raives, M. J., S. M. Couch, J. P. Greco, O. Pejcha, and T. A. Thompson. "The Antesonic Condition for the Explosion of Core-Collapse Supernovae – I. Spherically Symmetric Polytropic Models: Stability and Wind Emergence," *Monthly Notices of the Royal Astronomical Society* (September 2-18), Oxford University Press. doi:10.1093/mnras/sty2457.

Som, S., and Y. Pei. "HPC Opens a New Frontier in Fuel-Engine Research," *Computing in Science and Engineering* (September 2018), IEEE. doi:10.1109/mcse.2018.05329817.

Van Roekel, L., A. J. Adcroft, G. Danabasoglu, S. M. Griffies, B. K. Kauffman, W. Large, M. Levy, B. G. Reichl, T. Ringler, and M. Schmidt. "The KPP Boundary Layer Scheme for the Ocean: Revisiting Its Formulation and Benchmarking One-Dimensional Simulations Relative to LES," *Journal of Advances in Modeling Earth Systems* (September 2018), John Wiley and Sons. doi:10.1029/2018MS001336.

Vescovi, R., M. Du, V. de Andrade, W. Scullin, G. Gürsoy, and C. Jacobsen. "Tomosaic: Efficient Acquisition and Reconstruction of Teravoxel Tomography Data Using Limited-Size Synchrotron X-Ray Beams," *Journal of Synchrotron Radiation* (September 2018), International Union of Crystallography. doi:10.1107/s1600577518010093

Vidal, A., H. M. Nagib, P. Schlatter, and R. Vinuesa. "Secondary Flow in Spanwise-Periodic In-Phase Sinusoidal Channels," *Journal of Fluid Mechanics* (September 2018), Cambridge University Press. doi:10.1017/jfm.2018.498.

Zheng, Q., E. Xu, E. Park, H. Chen, and D. Shuai. "Looking at the Overlooked Hole Oxidation: Photocatalytic Transformation of Organic Contaminants on Graphitic Carbon Nitride under Visible Light Irradiation," *Applied Catalysis B: Environmental* (September 2018), Elsevier. doi:10.1016/j.apcatb.2018.09.012.

October

Asami, K., J. Ueda, K. Yasuda, K. Hongo, R. Maezono, M. G. Brik, and S. Tanabe. "Development of Persistent Phosphor of Eu^{2+} Doped Ba2SiO4 by Er^{3+} Codoping Based on Vacuum Referred Binding Energy Diagram," *Optical Materials* (October 2018), Elsevier. doi:10.1016/j.optmat.2018.07.021.

Bai, Z., N. H. Christ, X. Feng, A. Lawson, A. Portelli, and C. T. Sachrajda. "$K^+ \to \pi^+ \nu$ Decay Amplitude from Lattice QCD," *Physical Review D* (October 2018), APS. doi:10.1103/PhysRevD.98.074509.

Borsanyi, S., Z. Fodor, J. N. Guenther, S. K. Katz, A. Pasztor, I. Portillo, C. Ratti, and K. K. Szabó. "Higher Order Fluctuations and Correlations of Conserved Charges from Lattice QCD," *Journal of High Energy Physics* (October 2018), Springer Nature. doi:10.1007/JHEP10(2018)205.

Chang, H.-Y., A. Yazdani, X. Li, K. A. A. Douglas, C. S. Mantzoros, and G. E. Karniadakis. "Quantifying Platelet Margination in Diabetic Blood Flow," *Biophysical Journal* (October 2018), Elsevier. doi:10.1016/j.bpj.2018.08.031.

Feng, Y., Y. Zhao, W.-K. Zhou, Q. Li, W. A. Saidi, Q. Zhao, and X.-Z. Li. "Proton Migration in Hybrid Lead Iodide Perovskites: From Classical Hopping to Deep Quantum Tunneling," *The Journal of Physical Chemistry Letters* (October 2018), ACS. doi:10.1021/acs.jpclett.8b02929.

Fletcher, G., C. Bertoni, M. Keçeli, and M. D'Mello. "Valence: A Massively Parallel Implementation of the Variational Subspace Valence Bond Method," *ChemRxiv* (October 2018), ACS. doi:10.26434/chemrxiv.7439159.

Gladstein, S., L. M. Almassalha, L. Cherkezyan, J. E. Chandler, A. Eshein, A. Eid, D. Zhang, W. Wu, G. M. Bauer, A. D. Stephens, S. Morochnik, H. Subramanian, J. F. Marko, G. A. Ameer, I. Szleifer, and V. Backman. "Multimodal Interferometric Imaging of Nanoscale Structure and Macromolecular Motion Uncovers UV Induced Cellular Paroxysm," *bioRxiv* (October 2018), Cold Spring Harbor Laboratory. doi:10.1101/428383.

Järvi, J., J. Li, and P. Rinke. "Multi-Scale Model for the Structure of Hybrid Perovskites: Analysis of Charge Migration in Disordered MAPbI$_3$ Structures," *New Journal of Physics* (October 2018), IOP Publishing. doi:10.1088/1367-2630/aae295.

Jian, Y., S. Deng, S. Hong, J. Zhao, S. Huang, C.-C. Wu, J. L. Gottfried, K. Nomura, Y. Li, S. Tiwari, R. K. Kalia, P. Vashishta, A. Nakano, and X. Zheng. "Energetic Performance of Optically Activated Aluminum/Graphene Oxide Composites," *ACS Nano* (October 2018), ACS. doi:10.1021/acsnano.8b06217.

Kumar, P., and K. Mahesh. "Large-Eddy Simulation of Flow over an Axisymmetric Body of Revolution," *Journal of Fluid Mechanics* (October 2018), Cambridge University Press. doi:10.1017/jfm.2018.585.

Lee, C.-W., and A. Schleife. "Electronic Stopping and Proton Dynamics in InP, GaP, and In$_{0.5}$Ga$_{0.5}$P from First Principles," The European Physical Journal B (October 2018), Springer Nature. doi:10.1140/epjb/e2018-90204-8.

Lee, C.-W., and A. Schleife. "Novel Diffusion Mechanism in the Presence of Excited Electrons?: Ultrafast Electron-Ion Dynamics in Proton-Irradiated Magnesium Oxide," *Materials Today* (October 2018), Elsevier. doi:10.1016/j.mattod.2018.08.004.

Leistenschneider, E., M. P. Reiter, S. A. San Andrés, B. Kootte, J. D. Holt, P. Navrátil, C. Babcock, C. Barbieri, B. R. Barquest, J. Bergmann, J. Bollig, T. Brunner, E. Dunling, A. Finlay, H. Geissel, L. Graham, F. Greiner, H. Hergert, C. Hornung, C. Jesch, R. Klawitter, Y. Lan, D. Lascar, K. G. Leach, W. Lippert, J. E. McKay, S. F. Paul, A. Schwenk, D. Short, J. Simonis, V. Somà, R. Steinbrügge, S. R. Stroberg, R. Thompson, M. E. Wieser, C. Will, M. Yavor, C. Andreoiu, T. Dickel, I. Dillmann, G. Gwinner, W. R. Plaß, C. Scheidenberger, A. A. Kwiatkowski, and J. Dilling. "Dawning of the N=32 Shell Closure Seen through Precision Mass Measurements of Neutron-Rich Titanium Isotopes," *Physical Review Letters* (October 2018), APS. doi:10.1103/PhysRevLett.120.062503.

Li, N., S. Elhatisari, E. Epelbaum, D. Lee, B.-N. Lu, and U.-G. Meißner. "Neutron-Proton Scattering with Lattice Chiral Effective Field Theory at Next-to-Next-to-Next-to-Leading Order," *Physical Review C* (October 2018), APS. doi:10.1103/PhysRevC.98.044002.

Li, Y., N. A. Romero, and K. C. Lau. "Structure-Property of Lithium-Sulfur Nanoparticles via Molecular Dynamics Simulation," *ACS Applied Materials and Interfaces* (October 2018), ACS. doi:10.1021/acsami.8b09128.

Liu, C., W. Huhn, K.-Z. Du, Á. Vázquez-Mayagoitia, D. Dirkes, W. You, Y. Kanai, D. B. Mitzi, and V. Blum. "Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites," *Physical Review Letters* (October 2018), APS. doi:10.1103/physrevlett.121.146401.

McAvoy, R. L., M. Govoni, and G. Galli. "Coupling First-Principles Calculations of Electron-Electron and Electron-Phonon Scattering, and Applications to Carbon-Based Nanostructures," *Journal of Chemical Theory and Computation* (October 2018), ACS. doi:10.1021/acs.jctc.8b00728.

Mironov, V., Y. Alexeev, V. K. Mulligan, and D. G. Fedorov. "A Systematic Study of Minima in Alanine Dipeptide," *Journal of Computational Chemistry* (October 2018), John Wiley and Sons. doi:10.1002/jcc.25589.

Penchoff, D. A., C. C. Peterson, J. P. Camden, J. A. Bradshaw, J. D. Auxier II, G. K. Schweitzer, D. M. Jenkins, R. J. Harrison, and H. L. Hall. "Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes," *ACS Omega* (October 2018), ACS. doi:10.1021/acsomega.8b02068.

Sheng, C., S. Hong, A. Krishnamoorthy, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. "Role of H Transfer in the Gas-Phase Sulfidation Process of MoO$_3$: A Quantum Molecular Dynamics Study," *The Journal of Physical Chemistry Letters* (October 2018), ACS. doi:10.1021/acs.jpclett.8b02151.

Shields, C. A., J. J. Rutz, L. R. Leung, F. M. Ralph, M. Wehner, T. O'Brien, and R. Pierce. "Defining Uncertainties through Comparison of Atmospheric River Tracking Methods," *BAMS* (October 2018), American Meterological Society. doi:10.1175/BAMS-D-18-0200.1.

Šukys, J., U. Rasthofer, F. Wermelinger, P. Hadjidoukas, and P. Koumoutsakos. "Multilevel Control Variates for Uncertainty Quantification in Simulations of Cloud Cavitation," *SIAM Journal on Scientific Computing* (October 2018), SIAM. doi:10.1137/17m1129684.

Wakayama, H., K. Utimula, T. Ichibha, R. Kuriki, K. Hongo, R. Maezono, K. Oka, and K. Maeda. "Light Absorption Properties and Electronic Band Structures of Lead Titanium Oxyfluoride Photocatalysts Pb$_2$Ti$_4$O$_9$F$_2$ and Pb$_2$Ti$_2$O$_{5.4}$F$_{1.2}$," *The Journal of Physical Chemistry C* (October 2018), ACS. doi:10.1021/acs.jpcc.8b08953.

Zhai, X. M., and S. Kurien. "Characteristic Length Scales of Strongly Rotating Boussinesq Flow in Variable-Aspect-Ratio Domains," *Journal of Fluid Mechanics* (October 2018), Cambridge University Press. doi:10.1017/jfm.2018.687.

Zhang, H., R. Betti, R. Yan, D. Zhao, D. Shvarts, and H. Aluie. "Self-Similar Multimode Bubble-Front Evolution of the Ablative Rayleigh-Taylor Instability in Two and Three Dimensions," *Physical Review Letters* (October 2018), APS. doi:10.1103/PhysRevLett.121.185002.

Zhdankin, V., D. A. Uzdensky, G. R. Werner, and M. C. Begelman. "System-Size Convergence of Nonthermal Particle Acceleration in Relativistic Plasma Turbulence," *The Astrophysical Journal Letters* (October 2018), IOP Publishing. doi:10.3847/2041-8213/aae88c.

November

Blondel, S., D. E. Bernholdt, K. D. Hammond, and B. D. Wirth. "Continuum-Scale Modeling of Helium Bubble Bursting under Plasma-Exposed Tungsten Surfaces," *Nuclear Fusion* (November 2018), IOP Publishing. doi:10.1088/1741-4326/aae8ef.

Boyle, P., R. J. Hudspith, T. Izubuchi, A. Jüttner, C. Lehner, R. Lewis, K. Maltman, H. Ohki, A. Portelli, and M. Spraggs. "Novel |V_{us}| Determination Using Inclusive Strange τ Decay and Lattice Hadronic Vacuum Polarization Functions," *Physical Review Letters* (November 2018), APS. doi:10.1103/PhysRevLett.121.202003.

Cabezón, R. M., K.-C. Pan, M. Liebendörfer, T. Kuroda, K. Ebinger, O. Heinimann, A. Perego, and F.-K. Thielemann. "Core-Collapse Supernovae in the Hall of Mirrors: A Three-Dimensional Code-Comparison Project," *Astronomy and Astrophysics* (November 2018), EDP Sciences. doi:10.1051/0004-6361/201833705.

Cherukara, M. J., Y. S. G. Nashed, and R. J. Harder. "Real-Time Coherent Diffraction Inversion Using Deep Generative Networks," *Scientific Reports* (November 2018), Springer Nature. doi:10.1038/s41598-018-34525-1.

Du, M., R. Vescovi, K. Fezzaa, C. Jacobsen, and D. Gürsoy. "X-Ray Tomography of Extended Objects: A Comparison of Data Acquisition Approaches," *Journal of the Optical Society of America A* (November 2018), The Optical Society. doi:10.1364/josaa.35.001871.

Goth, N., P. Jones, D. T. Nguyen, R. Vaghetto, Y. A. Hassan, A. Obabo, E. Merzari, and P. F. Fischer. "Comparison of Experimental and Simulation Results on Interior Subchannels of a 61-Pin Wire-Wrapped Hexagonal Fuel Bundle," *Nuclear Engineering and Design* (November 2018), Elsevier. doi:10.1016/j.nucengdes.2018.08.002.

He, Y., K. Nomura, R. K. Kalia, A. Nakano, and P. Vashishta. "Structure and Dynamics of Water Confined in Nanopourous Carbon," *Physical Review Materials* (November 2018), APS. doi:10.1103/physrevmaterials.2.115605.

Hou, K., R. Al-Bahrani, E. Rangel, A. Agrawal, R. Latham, R. Ross, A. Choudhary, and W. Liao. "Integration of Burst Buffer in High-Level Parallel I/O Library for Exascale Era," *2018 IEEE/ACM 3rd International Workshop on Parallel Data Storage and Data Intensive Scalable Computing Systems* (November 2018), Dallas, TX, IEEE, doi:10.1109/PDSW-DISCS.2018.000-1.

Iwasaki, S., A. Amer, K. Taura, and P. Balaji. "Lessons Learned from Analyzing Dynamic Promotion for User-Level Threading," *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis* (November 2018), Dallas, TX, IEEE.

Jain, R., X. Luo, G. Sever, T. Hong, and C. Catlett. "Representation and Evolution of Urban Weather Boundary Conditions in Downtown Chicago," *Journal of Building Performance Simulation* (November 2018), Taylor and Francis Group. doi:10.1080/19401493.2018.1534275.

Lockwood, G. K., S. Snyder, T. Wang, S. Byna, P. Carns, and N. J. Wright. "A Year in the Life of a Parallel File System," *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis* (November 2018), Dallas, TX, IEEE.

Mahadevan, V. S., I. Grindeanu, R. Jacob, and J. Sarich. "Improving Climate Model Coupling through a Complete Mesh Representation: A Case Study with E3SM (v1) and MOAB (v5.x)," *Geoscientific Model Development* (November 2018), European Geosciences Union. doi:10.5194/gmd-2018-280.

Nathanson, M., K. Kanhaiya, A. Pryor Jr., J. Miao, and H. Heinz. "Atomic-Scale Structure and Stress Release Mechanism in Core-Shell Nanoparticles," *ACS Nano* (November 2018), ACS. doi:10.1021/acsnano.8b06118.

Shahbazi, A., J. Kinnison, R. Vescovi, M. Du, R. Hill, M. Joesch, M. Takeno, H. Zeng, N. Maçarico da Costa, J. Grutzendler, N. Kasthuri, and W. J. Scheirer. "Flexible Learning-Free Segmentation and Reconstruction of Neural Volumes," *Scientific Reports* (November 2018), Springer Nature. doi:10.1038/s41598-018-32628-3.

Sun, Z. H., T. D. Morris, G. Hagen, G. R. Jansen, and T. Papenbrock. "Shell-Model Coupled-Cluster Method for Open-Shell Nuclei," *Physical Review C* (November 2018), APS. doi:10.1103/PhysRevC.98.054320.

Wang, B., R. K. Kalia, A. Nakano, and P. D. Vashishta. "Dewetting of Monolayer Water and Isopropanol between MoS_2 Nanosheets," *Scientific Reports* (November 2018), Springer Nature. doi:10.1038/s41598-018-35163-3.

Withers, K. B., K. B. Olsen, S. M. Day, and Z. Shi. "Ground Motion and Intraevent Variability from 3D Deterministic Broadband (0–7.5 Hz) Simulations along a Nonplanar Strike-Slip Fault," *Bulletin of the Seismological Society of American* (November 2018), Seismological Soceity of America. doi:10.1785/0120180006.

Zhou, G., P. Rajak, S. Susarla, P. M. Ajayan, R. K. Kalia, A. Nakano, and P. Vashishta. "Molecular Simulation of MoS_2 Exfoliation," *Scientific Reports* (November 2018), Springer Nature. doi:10.1038/s41598-018-35008-z.

Zhu, E., S. Wang, X. Yan, M. Sobani, L. Ruan, C. Wang, Y. Liu, X. Duan, H. Heinz, and Y. Huang. "Long-Range Hierarchical Nanocrystal Assembly Driven by Molecular Structural Transformation," *Journal of the American Chemical Society* (November 2018), ACS. doi:10.1021/jacs.8b08023.

December

Alves, E. P., J. Zrake, and F. Fiuza. "Efficient Nonthermal Particle Acceleration by the Kink Instability in Relativistic Jets," *Physical Review Letters* (December 2018), APS. doi:10.1103/PhysRevLett.121.245101.

Appelquist, T., R. C. Brower, G. T. Fleming, A. Gasbarro, A. Hasenfratz, J. INgolby, J. Kiskis, J. C. Osborn, C. Rebbi, E. Rinaldi, D. Schaich, P. Vranas, E. Weinberg, and O. Witzel. "Linear Sigma EFT for Nearly Conformal Gauge Theories," *Physical Review D* (December 2018), APS. doi:10.1103/PhysRevD.98.114510.

Blondel, S., D. E. Bernholdt, K. D. Hammond, and B. D. Wirth. "Corrigendum: Continuum-Scale Modeling of Helium Bubble Bursting under Plasma-Exposed Tungsten Surfaces," *Nuclear Fusion* (December 2018), IOP Publishing. doi:10.1088/1741-4326/aaf330.

Bodling, A., and A. Sharma. "Numerical Investigation of Low-Noise Airfoils Inspired by the Down Coat of Owls," *Bioinspiration and Biomimetics* (December 2018), IOP Publishing. doi:10.1088/1748-3190/aaf19c.

Chen, J., E. Zhu, J. Liu, S. Zhang, Z. Lin, X. Duan, H. Heinz, Y. Huang, and J. J. De Yoreo. "Building Two-Dimensional Materials One Row at a Time: Avoiding the Nucleation Barrier," *Science* (December 2018), AAAS. doi:10.1126/science.aau4146.

Chen, Z., S. E. Boyken, M. Jia, F. Busch, D. Flores-Solis, M. J. Bick, P. Lu, Z. L. VanAernum, A. Sahasrabuddhe, R. A. Langan, S. Bermeo, T. J. Brunette, V. K. Mulligan, L. P. Carter, F. DiMaio, N. G. Sgourakis, V. H. Wysocki, and D. Baker. "Programmable Design of Orthogonal Protein Heterodimers," *Nature* (December 2018), Springer Nature. doi:10.1038/s41586-018-0802-y.

Cooper, C. B., E. J. Beard, Á. Vázquez-Mayagoitia, L. Stan, G. B. B. Stenning, D. W. Nye, J. A. Vigil, T. Tomar, J. Jia, G. B. Bodedla, S. Chen, L. Gallego, S. Franco, A. Carella, K. R. J. Thomas, S. Xue, X. Zhu, and J. M. Cole. "Design-to-Device Approach Affords Panchromatic Co-Sensitized Solar Cells," *Advanced Energy Materials* (December 2018), John Wiley and Sons. doi:10.1002/aenm.201802820.

Jin, Z., and H. Finkel. "Optimizing Radial Basis Function Kernel on OpenCL FPGA Platform," *2018 IEEE International Conference on Big Data* (December 2018), Seattle, WA, IEEE. doi:10.1109/BigData.2018.8622219.

Kar, M., and T. Körzdörfer. "Computational Screening of Methylammonium Based Halide Perovskites with Bandgaps suitable for Perovskite-Perovskite Tandem Solar Cells," *The Journal of Chemical Physics* (December 2018), AIP. doi:10.1063/1.5037535.

Le, T. B., A. Khosronejad, F. Sotiropoulos, N. Bartelt, S. Woldeamlak, and P. Dewall. "Large-Eddy Simulation of the Mississippi River under Base-Flow Condition: Hydrodynamics of a Natural Diffluence-Confluence Region," *Journal of Hydraulic Research* (December 2018), Taylor and Francis Group. doi:10.1080/00221686.2018.1534282.

Li, J., M. Otten, A. A. Holmes, S. Sharma, and C. J. Umrigar. "Fast Semistochastic Heat-Bath Configuration Interaction," *The Journal of Chemical Physics* (December 2018), AIP. doi:10.1063/1.5055390.