Argonne
NATIONAL LABORATORY
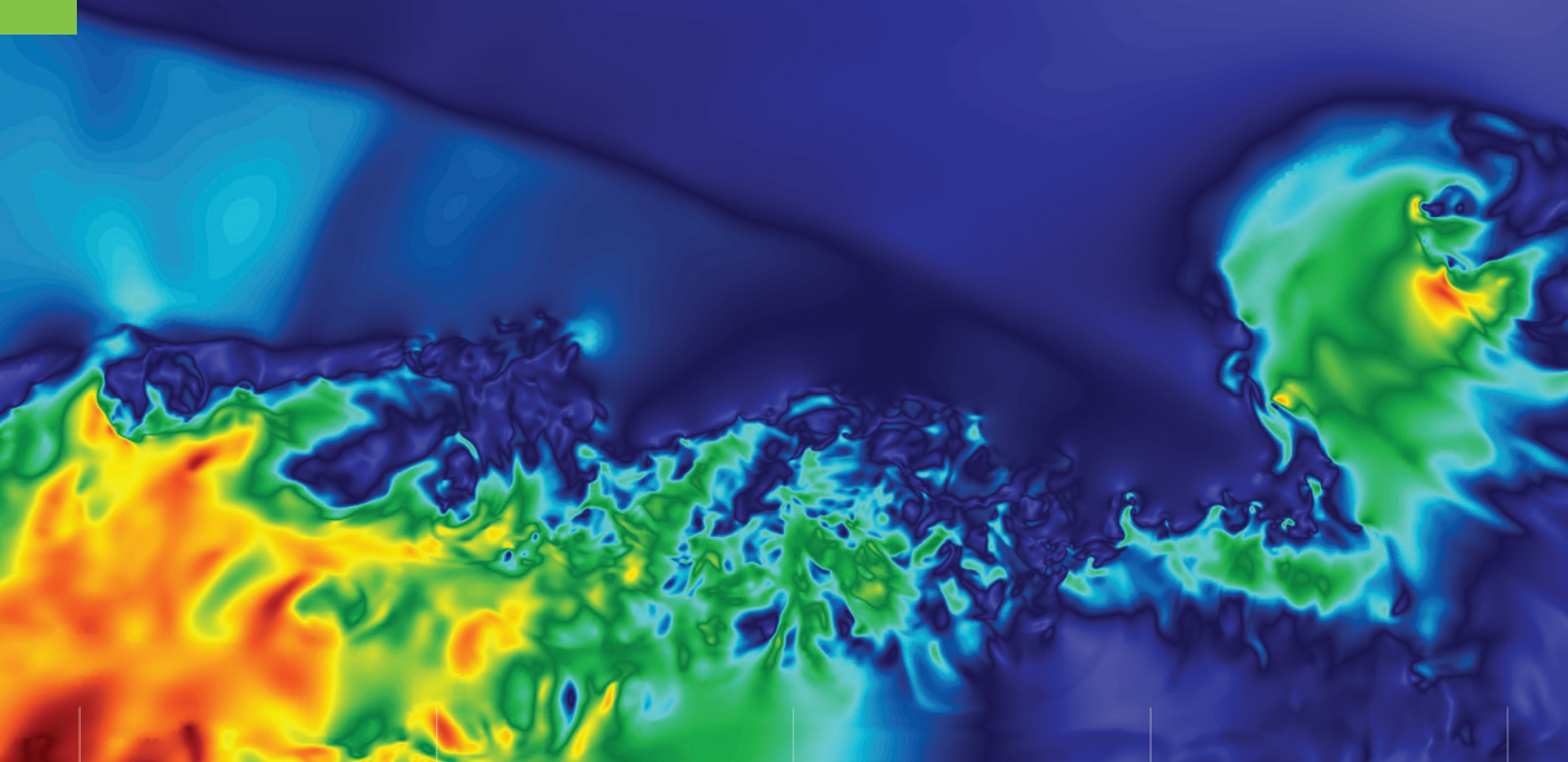
2015 ANNUAL REPORT
ARGONNE LEADERSHIP COMPUTING FACILITY

ARGONNE LEADERSHIP COMPUTING FACILITY

ANNUAL REPORT 2015

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ABOUT ALCF

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

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

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

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

DIRECTOR'S MESSAGE

2015 marked 10 years since Argonne installed its first IBM Blue Gene system—a 5-teraflops machine that was both a prototype and a proving ground for what would become the Argonne Leadership Computing Facility in 2006. The BG/L was the latest in a long line of parallel computing systems that Argonne mathematicians and computer scientists procured and experimented with starting in the early 1980s.

That same machine supported the first six Department of Energy (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) projects at Argonne, and solidified a decade-long industry partnership that has produced some of the world's most powerful machines supporting high-end computational science and engineering.

Today, ALCF's main resource, Mira, an IBM Blue Gene/Q, is *2,000 times* more powerful than Argonne's BG/L. It is the last in a very successful series of computers on which the research community has solved some of the most pressing problems facing our planet. And now we look to the future.

Of course, it was big news in 2015 when DOE announced Argonne's next-generation systems. The 180-petaflops supercomputer, known as Aurora, is planned to arrive in 2018, and will be a massively many-core system based on Intel's Knights Hill Xeon Phi processor technology and integrated on Cray's next-generation hardware platform. Preceding Aurora's arrival is Theta, based on Intel's Knights Landing technology, slated for installation in late 2016.

In 2015, the ALCF supported 34 INCITE projects, 25 ASCR Leadership Computing Challenge projects, and more than 190 Director's Discretionary projects. The facility also provided short-term strategic computational runs to science teams working in other major facilities to run analysis jobs on their data-intensive experiments. These included high-energy x-ray beamline teams, a partnership pursuing breakthroughs in battery research, and physicists using the world's most powerful particle accelerator— all of which are described in the following pages.

On the technical side, ALCF researchers made progress on several efforts, such as GLEAN and AutoPerf, aimed at improving high-performance computing (HPC) in leadership-class facilities and beyond. The operations team launched Cooley, a powerful new visualization and analysis cluster with terabytes of RAM and GPU memory

Michael E. Papka
Division Director, ALCF;
Deputy Associate Laboratory Director,
Computing, Environment, and Life Sciences

to help meet our user community's data analysis needs. Cooley, the follow-on system to Tukey, will support more exploration capabilities, including *in-situ* analysis and unprecedented volume-rendered visualization.

On the outreach side, ALCF staff promoted our services and world-class technical expertise within the HPC community, and continued to build on our successful training programs for our current and future users alike. The ALCF has hit its stride in many areas, and will no doubt continue to impact the greater HPC community through its research publications, software releases, and active involvement in standards bodies and working groups.

Our staff remains the ALCF's most valuable asset, and in this year's report we showcase a diversity of them: computational scientists Marta García and Chris Knight, application performance engineer Scott Parker, operations team lead Skip Reddy, postdoc and visualization expert Silvio Rizzi, and UX developer Savannah French. 2015 also saw major leadership changes, with Katherine Riley replacing Paul Messina as our second Director of Science, and Mark Fahey replacing Bill Allcock as our second Director of Operations.

This is my final annual letter to you as ALCF's director. After more than five years as director, I am returning to my full-time role as Argonne's Deputy Associate Laboratory Director for Computing, Environment, and Life Sciences, where I will continue to cultivate and support efforts that connect computing to areas of inquiry. I'm proud of the time I've spent at the ALCF and all the things the division has accomplished. I look forward to sharing in its future successes.

Michael E. Papka

ALCF LEADERSHIP: YEAR IN REVIEW

FUTURE SYSTEMS AND FACILITY INITIATIVES

Susan Coghlan
Deputy Director

In April, DOE's announcement of our two future systems, Theta and Aurora, made national news. The contracts to design and build the supercomputers were awarded to Intel and Cray. Like Mira, both machines will be many-core, homogeneous systems, which will help users with the transition from our current IBM architecture to the Intel Xeon Phi architecture. We continued to work diligently behind the scenes to prepare for the arrival of the new systems, making progress with facility enhancements to address their power and cooling requirements. In addition, we kicked off our Early Science Program for Theta and we began working closely with Intel and Cray to evaluate early hardware and to improve the system software.

SCIENCE

Katherine Riley
Director of Science

In October, I was named the ALCF's new Director of Science, the second in the facility's history. I'm excited about my role in shaping the ALCF's future as a world-class scientific computing center. We started phase one of our Early Science Program this year to help ready our new machines for science. The selected projects will also lead the way in demonstrating how applications can prepare for many of the architectural features we will see as we move toward exascale. In September, I chaired DOE's High-Performance Computing Operations Review (HPCOR) to identify ways to improve application portability on future systems. We also collaborated with OLCF and NERSC on the first two Exascale Requirements Reviews, which aim to determine the future computational science objectives for the six DOE Office of Science programs. Finally, Mira continued to enable our users to produce amazing science and engineering research, resulting in many high-impact publications.

OPERATIONS

Mark Fahey
Director of Operations

In my first year as ALCF Director of Operations, I'm pleased to report that Mira had its best performance year ever in 2015 — hitting or exceeding all key metrics for availability and utilization. We also installed a new visualization and analysis cluster with 386 GB of memory and a GPU per node, called Cooley, and decommissioned its predecessor. To improve our archival storage, we completed the swap of roughly 10,000 LTO4 tapes to LTO6 tapes, providing nearly three times the capacity. In collaboration with Argonne's Joint Laboratory for System Evaluation (JSLE), we piloted a data management service called Petrel that allows researchers to store and share large datasets internally and externally. This effort involved performing upgrades to the JLSE network, which resulted in 40/56 Gb Ethernet connectivity. In addition, we deployed a suite of tools to track compiler and library usage on our Blue Gene/Q systems. In the coming year, we will be deploying a new Cray XC system, a new "burst buffer-like" storage cache, a hierarchical storage management disk-to-tape migration solution, and a new allocation charging system.

USER EXPERIENCE

Richard Coffey
Director of User Experience

We have many evolving practices in place to help ensure a smooth and successful user experience at the ALCF. From day one, the user experience team interacts with the project teams nearly continuously; from helping them quickly gain access to the resources to providing training to promoting their accomplishments. In 2015, we exceeded all targets related to user support and problem resolution. We had our best-ever response rate for our annual user survey. We designed and executed our first-ever "Ensemble Jobs for Better Throughput" videoconference. And, I'm especially proud to report, every one of our 2016 INCITE projects were ready for prime time two weeks prior to the critical January 1 start date. All of the efforts helped remove roadblocks and enable scientists to focus on their research. I look forward to the challenges ahead. Great service is our goal and we never tire of finding solutions to problems.

PERFORMANCE ENGINEERING

Kalyan Kumaran
Manager, Performance Engineering

We had a very busy year, supporting users on Mira while also playing a critical technical role in preparations for our next-generation systems, Theta and Aurora. One of the highlights involving our current systems was the deployment of AutoPerf, a library that automatically collects performance data from applications. This tool is already proving to be tremendously helpful in our efforts to optimize applications and understand their requirements. For our future systems, we helped complete the non-recurring engineering (NRE) and build contracts and led NRE working groups to ensure that the new technologies meet the needs of the facility and our users. Our team also began porting applications and benchmarks to early hardware to reveal information on the Intel Xeon Phi architecture that will help ease the transition from Mira to Theta. In addition, we are leading a Theta Early Science Program project to port performance tools, debuggers, libraries, and other software to Theta to make them available when the system enters production mode next year.

VISUALIZATION AND DATA ANALYSIS

Mark Hereld
Manager, Visualization and Data Analysis

In June, we launched our new visualization and analysis platform, Cooley. With eight times the memory capacity of its predecessor, Tukey, Cooley improved our ability to visualize, delve into, and interact with large-scale numerical datasets. For instance, the new system enabled an INCITE team to perform massive 3D visualizations of high-speed combustion and detonation that were intractable on Tukey. In addition to helping scientists better understand and present their simulation results, Cooley also generated some visualizations that garnered noteworthy attention. We worked with an INCITE research team to produce a visualization of superlubricity that went on to be featured on the cover of DOE Quadrennial Technology Review. We also worked with Argonne engine researchers to generate a gasoline compression ignition visualization that was recognized as a finalist in the SC15 Visualization Showcase. We are looking forward to another year of helping our users to achieve research goals by turning their simulation data into illuminating visualizations.

AURORA AND

In April, DOE announced its investment to deliver Aurora and Theta, the ALCF's next-generation supercomputers.
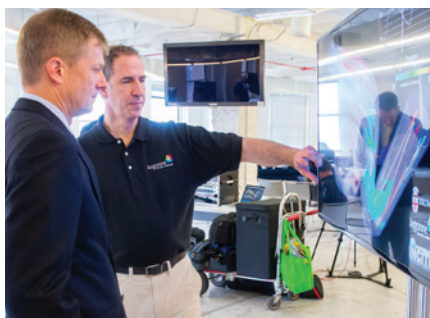
Top: ALCF visualization expert Joe Insley explains a blood flow simulation to a guest following the April 9 press event announcing Aurora and Theta.

Bottom: Argonne Director Peter Littlewood addresses the press and invited guests during the DOE announcement.

Designed in collaboration with industry leaders Intel and Cray, Aurora is scheduled for delivery in 2018. The effort is the result of DOE's Collaboration of Oak Ridge, Argonne, and Lawrence Livermore (CORAL) initiative, a joint procurement activity launched in 2014.

Aurora will deliver more than 18 times the computational performance of Mira, its predecessor at the ALCF, using a nearly equal number of compute nodes. Aurora will be a many-core system, but with nearly an order of magnitude more processors.

Aurora's revolutionary architecture features Intel's HPC scalable system framework and second-generation Intel® Omni-Path Fabric, providing a peak performance of 180 petaflops. The system will have a combined total of over 7 petabytes of on-package high-bandwidth memory and persistent memory,
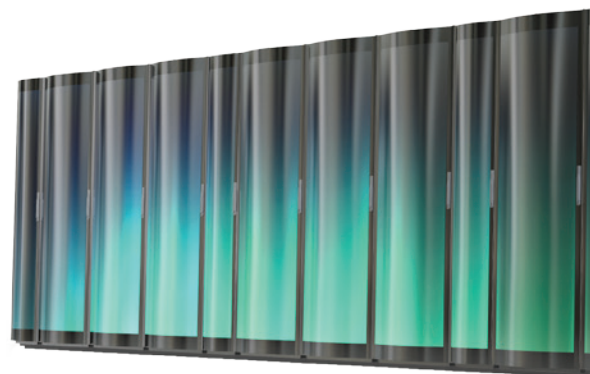
THETA

connected and communicating via a high-performance system fabric to achieve landmark throughput. The nodes will be linked to a dedicated burst buffer and a high-performance parallel storage solution.

The system will help ensure continued U.S. leadership in high-end computing for scientific research, while also cementing the nation's position as a global leader in the development of next-generation exascale computing systems.

A second system, named Theta, will be delivered in 2016 to serve as a bridge between Mira and Aurora. Based on Intel's second-generation Xeon Phi processor, Theta will enable breakthrough science and engineering research while providing an early production system to help ALCF users transition their applications to the new technology.

18x
FASTER

PREPARING THETA FOR SCIENCE ON DAY ONE

As part of the process of bringing a new supercomputer into production, the ALCF conducts the Early Science Program (ESP) to ensure its next-generation systems are ready to hit the ground running.

In August, the facility kicked off its Theta ESP with the selection of six computational science projects to help prepare scientific applications for the architecture and scale of the new supercomputer.

The ESP brings together computational scientists, code developers, and computing hardware experts to optimize key applications for Theta, and to solidify libraries and infrastructure to pave the way for other applications to run on the system.

Modeled after the ALCF's highly successful ESP for Mira, the program also gives researchers substantial allocations of pre-production compute time on Theta to pursue innovative computational science calculations that push the boundaries of what's possible with leadership-class supercomputers.
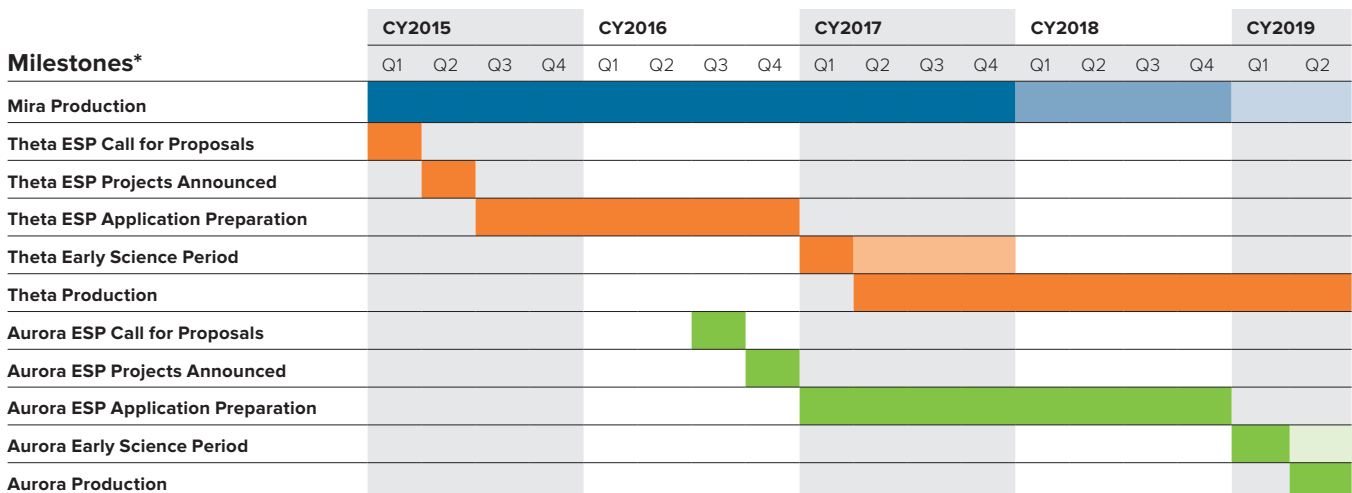
Like the typical ALCF workload, the six selected ESP projects, known as Tier One projects, represent a wide spectrum of scientific areas and numerical methods.To help develop and optimize their software for Theta, project teams are collaborating with ALCF and vendor staff. Four of the six projects were also assigned a dedicated postdoctoral researcher.

Because of the strong response to the call for proposals, the ALCF expanded the Theta ESP to include six additional Tier Two projects to help prepare other applications for Theta. While these projects did not receive allocations for science runs, they do have access to ESP training, an ESP discussion forum, early hardware, and to Theta itself for porting, tuning, and debugging. In addition, the ALCF is leading an omnibus ESP project to

port and adapt software tools, such as programming models, performance tools, debuggers, and libraries, so they are available during the system's early deployment phase.

Once Theta is delivered and accepted, the Early Science period will give ESP teams dedicated access to the full system before Theta enters production mode. The Theta ESP will culminate with a community workshop, open to all ALCF users, in which the project teams present their code development work and share lessons learned.

From Mira to Aurora

Milestones*	CY2015				CY2016				CY2017				CY2018				CY2019	
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2
Mira Production	█	█	█	█	█	█	█	█	█	█	█	█	▒	▒	▒	▒	░	░
Theta ESP Call for Proposals	█																	
Theta ESP Projects Announced		█																
Theta ESP Application Preparation			█	█	█	█	█	█										
Theta Early Science Period									█	▒	▒	▒	▒					
Theta Production										█	█	█	█	█	█	█	█	█
Aurora ESP Call for Proposals							█											
Aurora ESP Projects Announced								█										
Aurora ESP Application Preparation									█	█	█	█	█	█	█	█		
Aurora Early Science Period																	█	▒
Aurora Production																		█

* Dates are subject to change.

# Theta ESP Tier One Science Projects
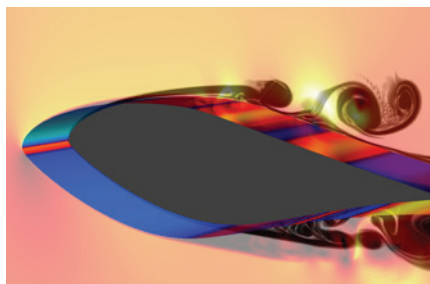
Scale-Resolving Simulations of Wind Turbines with SU2

Juan J. Alonso
Stanford University
Code: SU2

Researchers will develop a simulation capability to design better wind turbines and to lay out large wind farms for maximum energy extraction and improved turbine fatigue life. To do so, the research team will generate a database of large-eddy simulations of various single and multiple wind turbine settings.

Image credit: Ramesh Balakrishnan, Argonne National Laboratory
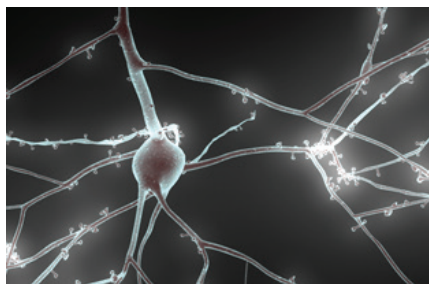
Large-Scale Simulation of Brain Tissue: Blue Brain Project, EPFL

Fabien Delalondre
EPFL
Code: CoreNeuron

This project aims to improve our understanding of the brain using simulations of brain plasticity—experience-dependent changes in synaptic connectivity. Other work will include simulating rodent somatosensory cortex and the electrical activity of the largest possible brain model for several seconds of biological time.

Image credit: Blue Brain Project, EPFL
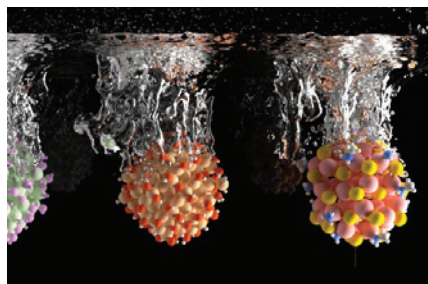
First-Principles Simulations of Functional Materials for Energy Conversion

Giulia Galli
The University of Chicago
Codes: Qbox, WEST

Researchers will combine *ab initio* molecular dynamics and post-density functional theory methods to optimize properties of nanostructured materials for use in solar and thermal energy conversion devices at an unprecedented level of accuracy. The ultimate goal is to provide a truly predictive tool for device performance within a Materials Genome Initiative design framework.

Image credit: Nicholas Brawand, The University of Chicago
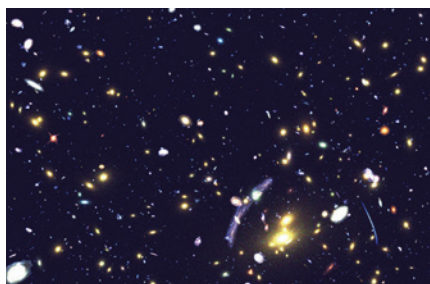
Next-Generation Cosmology Simulations with HACC: Challenges from Baryons

Katrin Heitmann
Argonne National Laboratory
Code: HACC

This project aims to further our understanding of astrophysical processes by performing detailed simulations of the universe for comparison with the latest observational data. The simulations will disentangle astrophysical processes (e.g., galaxy evolution) from fundamental physics (e.g., dark energy), helping mitigate one of the major sources of systematic uncertainties for upcoming cosmological surveys.

Image credit: Lindsey Bleem, Nan Li, and the HACC team, Argonne National Laboratory; Mike Gladders, The University of Chicago
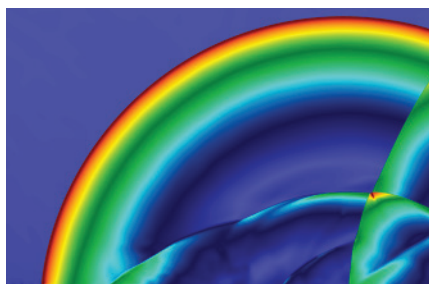

Direct Numerical Simulations of Flame Propagation in Hydrogen-Oxygen Mixtures in Closed Vessels

Alexei Khokhlov
The University of Chicago
Code: HSCD

Researchers will perform direct numerical simulations of the flame acceleration and the deflagration-to-detonation transition process in hydrogen-oxygen mixtures in closed spherical vessels—exactly matching experimental apparatus. This research is aimed at improving the industrial and public safety of hydrogen fuels and certain water-cooled nuclear reactors.

Image credit: Charles Bacon, Marta García, and Joseph A. Insley, Argonne National Laboratory; Alexei Khokhlov, The University of Chicago; Joanna Austin and Andrew Knisely, University of Illinois at Urbana-Champaign
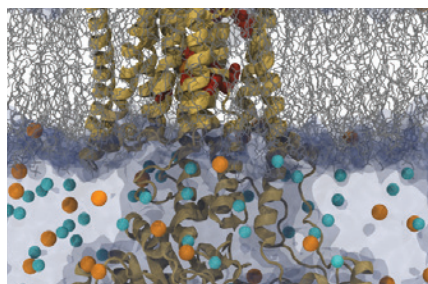
Free Energy Landscapes of Membrane Transport Proteins

Benoît Roux
The University of Chicago
Code: NAMD

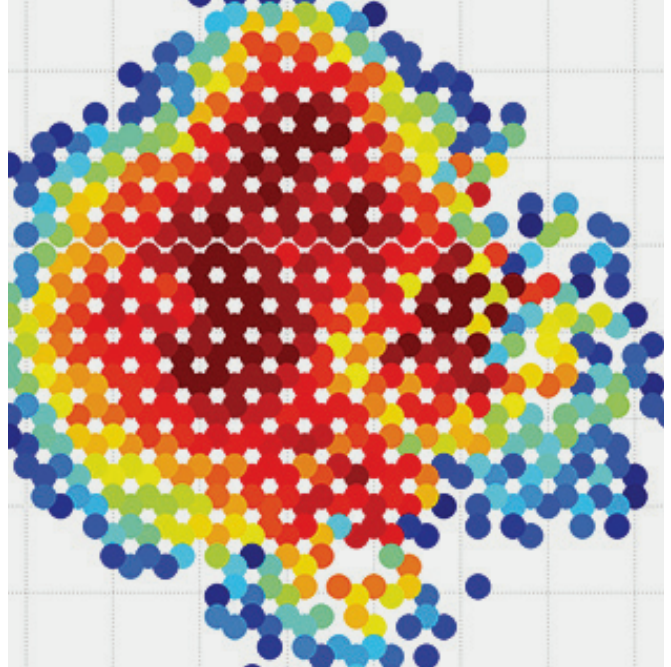This project will carry out molecular dynamics simulations to provide detailed visualizations of the large conformational changes of membrane transport proteins and quantitative predictions of the energetics of these processes. This atomistic picture of membrane transport proteins stands to improve our understanding of a broad range of biological functions.

Image credit: Brian Radak and Huan Rui, The University of Chicago

High-energy x-ray diffraction microscopy image of an ~50 micron diameter gold wire (courtesy of B. Suter, Carnegie Mellon University) showing confidence index for each ~1 micron voxel. The data is from the 1-ID beamline of the APS. Reconstructions conducted using APS and ALCF resources were led by Argonne researchers Hemant Sharma and Justin Wozniak.
Image credit: Jonathan Almer and Hemant Sharma, Argonne National Laboratory

ALCF RESOURCES PROPEL DATA-INTENSIVE EXPERIMENTS

Simulations have become an essential part of experimental research, providing information to help scientists test theories, understand results from experiments, and inform the setup of new experiments.

In 2015, the ALCF continued to build partnerships with experimental facilities that have large computation and data science challenges. The following collaborative efforts demonstrate how leadership computing resources can be used to propel scientific breakthroughs, and inform and facilitate large-scale, data-driven experiments.

Advanced Photon Source

Recent work by a collaboration of scientists from Argonne's Advanced Photon Source (APS), Mathematics and Computer Science (MCS) Division, and the ALCF has produced advances in computational methods and infrastructure that are helping to boost APS beamline performance.

As part of a high-energy diffraction microscopy (HEDM) project, a research team received a three-day allocation of APS beam time to develop new experimental techniques and algorithms to image the grain structures of polycrystalline materials. They also received a Director's Discretionary allocation at the ALCF to run an analysis job of their experimental procedure on Mira. Using the Swift parallel scripting language, MCS and ALCF researchers helped transform their HEDM analysis software into a scalable application capable of utilizing Mira efficiently.

The resulting simulations showed obviously skewed data, which allowed the APS researchers to adjust the experimental hardware and take new trial images until the confidence levels indicated a correct physical setup. The culprit was a cable that was too short, constraining the detector's movement. Without such in-beam experimentation and computational assessment, the researchers' beam time would have proceeded to completion, yielding useless data that would be discovered weeks or months later during a manual data analysis phase. By using Mira to help detect and correct a problem early on, the three-day experiment instead produced publishable results.
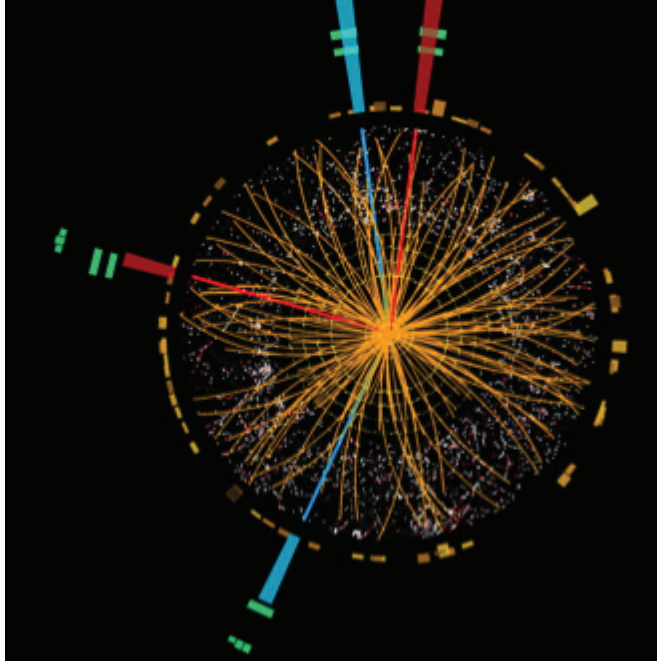
A Higgs → ZZ* candidate event from the ATLAS detector, showing the particle tracks and jets that require simulations to interpret.
Image credit: ATLAS Collaboration
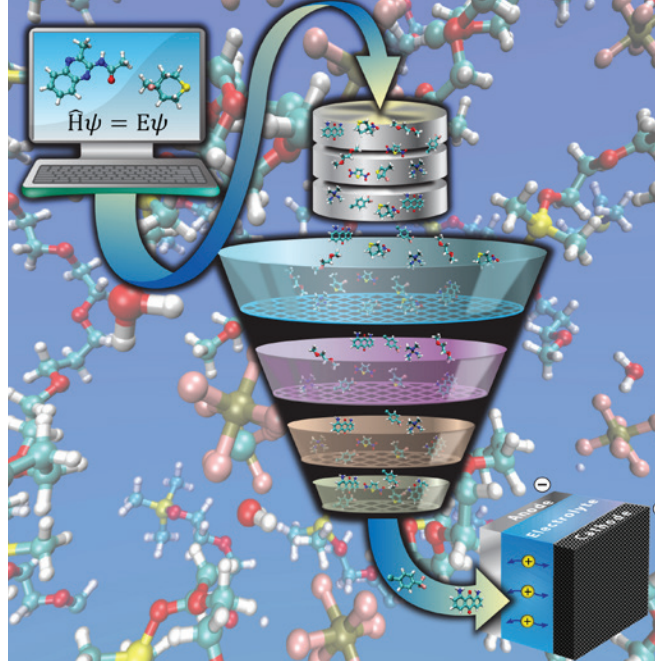
The Electrolyte Genome is a promising approach for evaluating vast libraries of electrolyte materials to inform and accelerate experimental efforts.
Image credit: Lei Cheng, Argonne National Laboratory

Large Hadron Collider

At CERN's Large Hadron Collider (LHC), scientists initiate millions of particle collisions every second in their quest to understand the fundamental structure of matter. Each collision produces about a megabyte of data. Even after filtering out about 99 percent of the data, scientists are left with around 30 petabytes each year to analyze for a wide range of physics experiments.

To help tackle the considerable challenge of interpreting all this data, Argonne physicists used an ALCC allocation to perform simulations of LHC experiments with a leadership-class supercomputer for the first time. ALCF researchers worked with the team to optimize the ALPGEN code for Mira, transforming it into multithreaded code that could take advantage of the petascale supercomputer's massively parallel architecture. The optimizations allowed the researchers to simulate complex particle collision events that were difficult to carry out on the LHC's computing grid. In fact, they were able to complete two years' worth of ALPGEN simulations in a matter of weeks.

The project is showing that supercomputers like Mira can help drive future discoveries at the LHC by accelerating the pace at which simulated data can be produced. The effort also demonstrates how leadership computing resources can be used to advance other data-intensive high energy physics experiments.

Joint Center for Energy Storage Research

Led by Argonne, the Joint Center for Energy Storage Research (JCESR) is a major DOE research partnership that integrates government, academic, and industrial researchers from many disciplines to overcome critical scientific and technical barriers and create new breakthrough energy storage technology. One of the center's projects, the Electrolyte Genome, relies on high-performance computers to sift through thousands of potential electrolyte materials to identify promising candidates for further research and development.

With a Director's Discretionary allocation, JCESR researchers gained access to ALCF computing resources, which provide the computational power needed to screen the vast possible space of electrolyte solvents, salts, and redox active combinations, and to perform mobility calculations for promising cathodes. ALCF researchers are working closely with the JCESR team to help adapt their code—the FireWorks workflow management software running Q-Chem's implementation of density functional theory—to perform accurately and efficiently on ALCF supercomputers.

Thus far, they have identified and resolved a variety of bugs and technical challenges to vastly improve the performance of Q-Chem on IBM Blue Gene/Q systems. JCESR scientists have successfully screened an initial pilot of 6,000 small molecules and now have the ability to virtually screen much larger molecules thanks to the computing infrastructure being developed as a part of this collaborative project.

ALLOCATION PROGRAMS

Any researcher in the world with a large-scale computing problem can apply for time on ALCF computing resources.

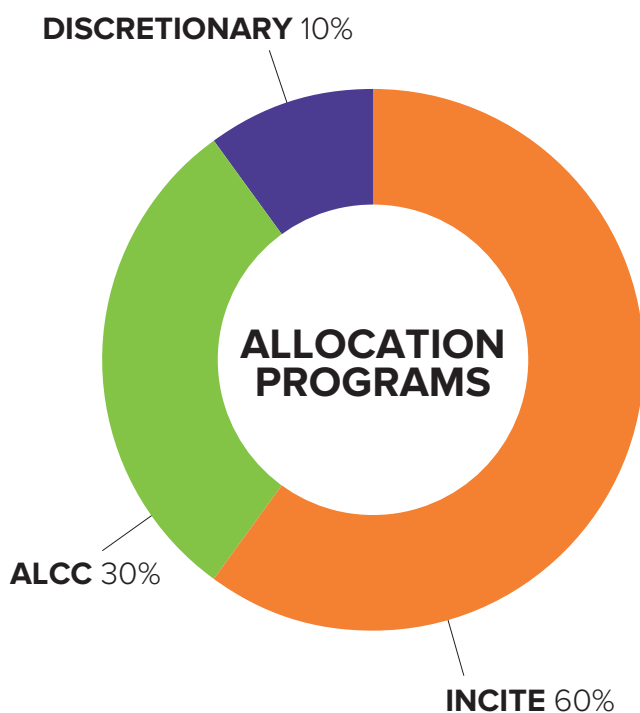### Innovative & Novel Computational Impact on Theory and Experiment (INCITE)

The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering. The program conducts a two-part review of all proposals: a peer review by an international panel of experts and a computational-readiness review. The annual call for proposals is issued in April, and the allocations are awarded in millions of core-hours for one to three years.

ASCR Leadership Computing Challenge (ALCC)

The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, national emergencies, or for broadening the community of researchers capable of using leadership computing resources. The DOE conducts a peer review of all proposals based on scientific and technical merit of the project; appropriateness of the proposed method or approach; competency and adequacy of personnel and proposed resources; and the reasonableness and appropriateness of the proposed allocation request. The yearlong allocation cycle runs from July 1 to June 30.

Director's Discretionary

The ALCF's Director's Discretionary program provides "start up" awards to researchers working toward an INCITE or ALCC allocation to help them achieve computational readiness. Projects must demonstrate a need for leadership-class resources. Awards may be made year round to industry, academia, laboratories, and others, and are usually between three and six months in duration. The size of the award varies based on the application and its readiness/ability to scale; awards are generally from the low hundreds of thousands to the low millions of core-hours.

DISCRETIONARY 10%

ALLOCATION PROGRAMS

ALCC 30%

INCITE 60%

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

2015 INCITE
BY DOMAIN

3.57 BILLION
CORE-HOURS

Computer Science 2%
Biological Sciences 5%
Chemistry 8%
Earth Science 13%
Engineering 15%
Materials Science 29%
Physics 28%

2015 ALCC
BY DOMAIN

1.74 BILLION
CORE-HOURS

Computer Science 6%
Biological Sciences 6%
Earth Science 7%
Chemistry 11%
Materials Science 19%
Physics 31%
Engineering 20%
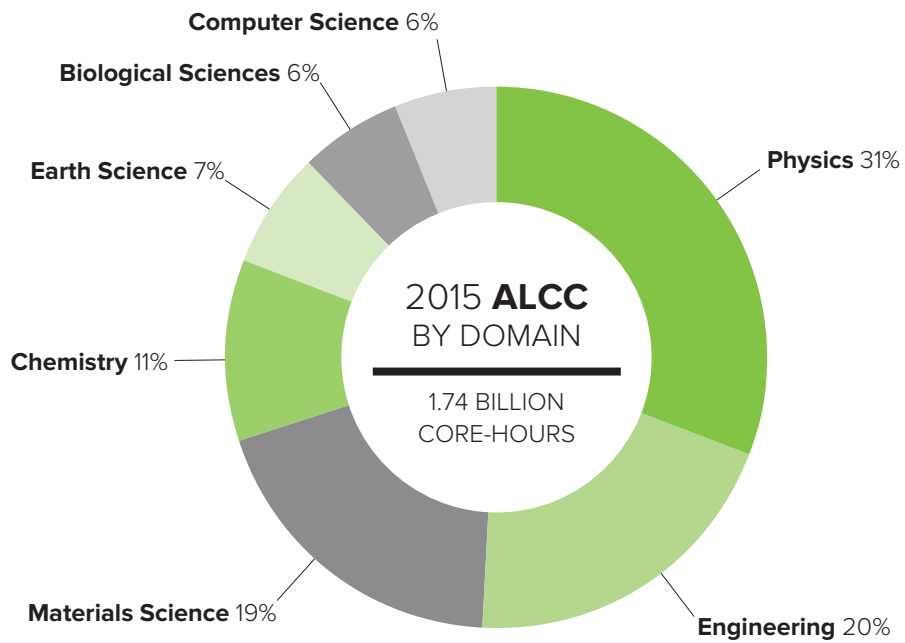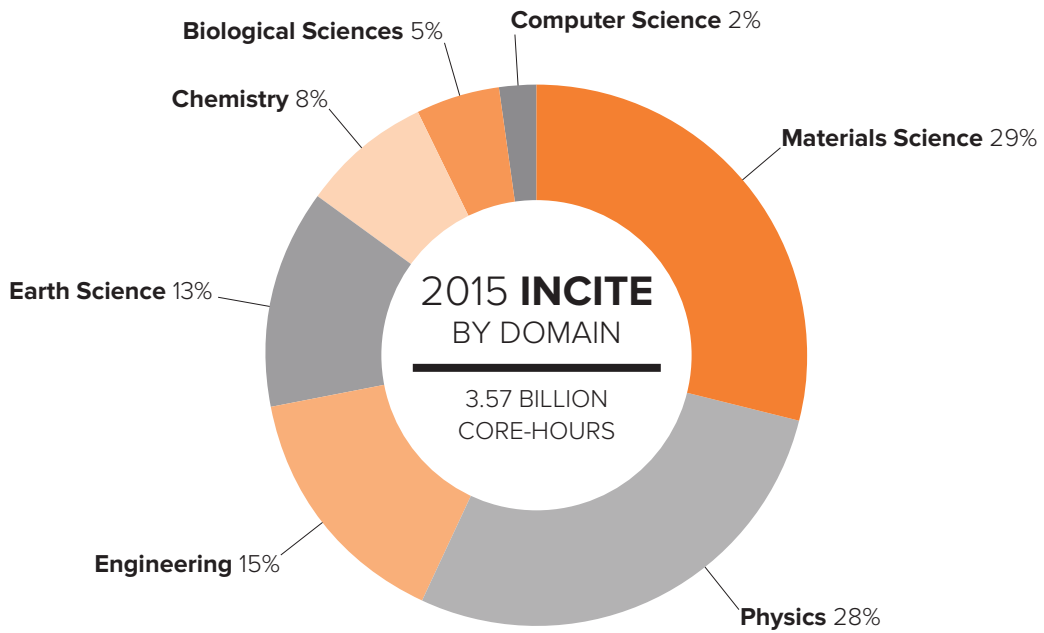
Note: Data is from calendar year 2015.

2015 MIRA USAGE
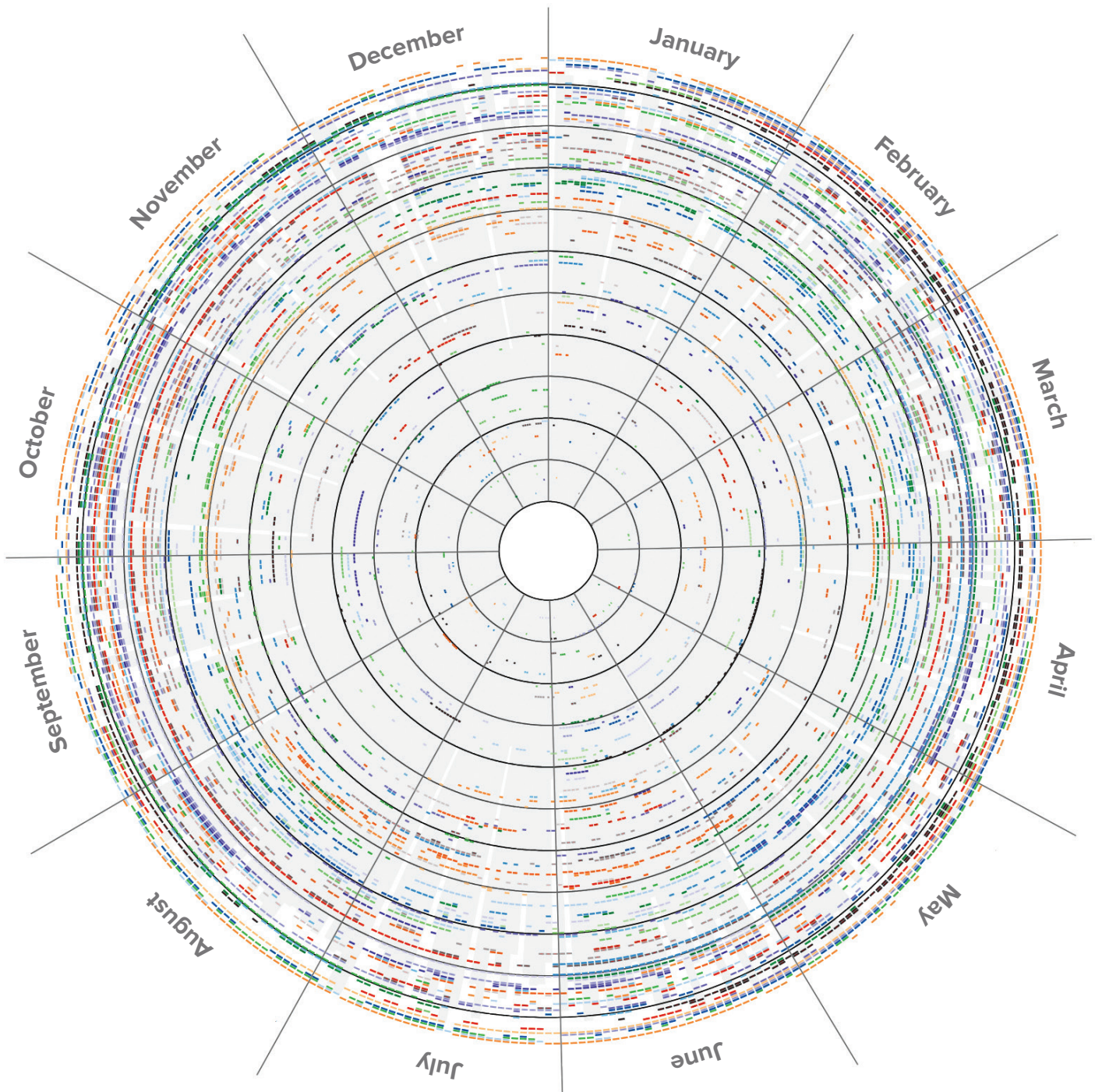
This visualization depicts all projects and jobs that ran on Mira in 2015. Each colored ring represents a project; each box represents a day that the project ran a job on the system. The radial histogram in the background shows the percentage of overall machine usage for that day (with 0 percent at the inner circle and 100 percent at the outer edge of the circle).

Image credit: Michael E. Papka and Eric Pershey, Argonne National Laboratory; Adam Young, Northern Illinois University

This figure displays streamlines of the two-dimensional skin friction field which was obtained right at the heated bottom plate of a cylindrical cell for turbulent Rayleigh-Bénard convection in liquid mercury at a Rayleigh number of a hundred million. The field displays the complex dynamics of the velocity field.

Image credit: Joerg Schumacher, Technische Universitaet Ilmenau

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

SCIE

SCIENCE
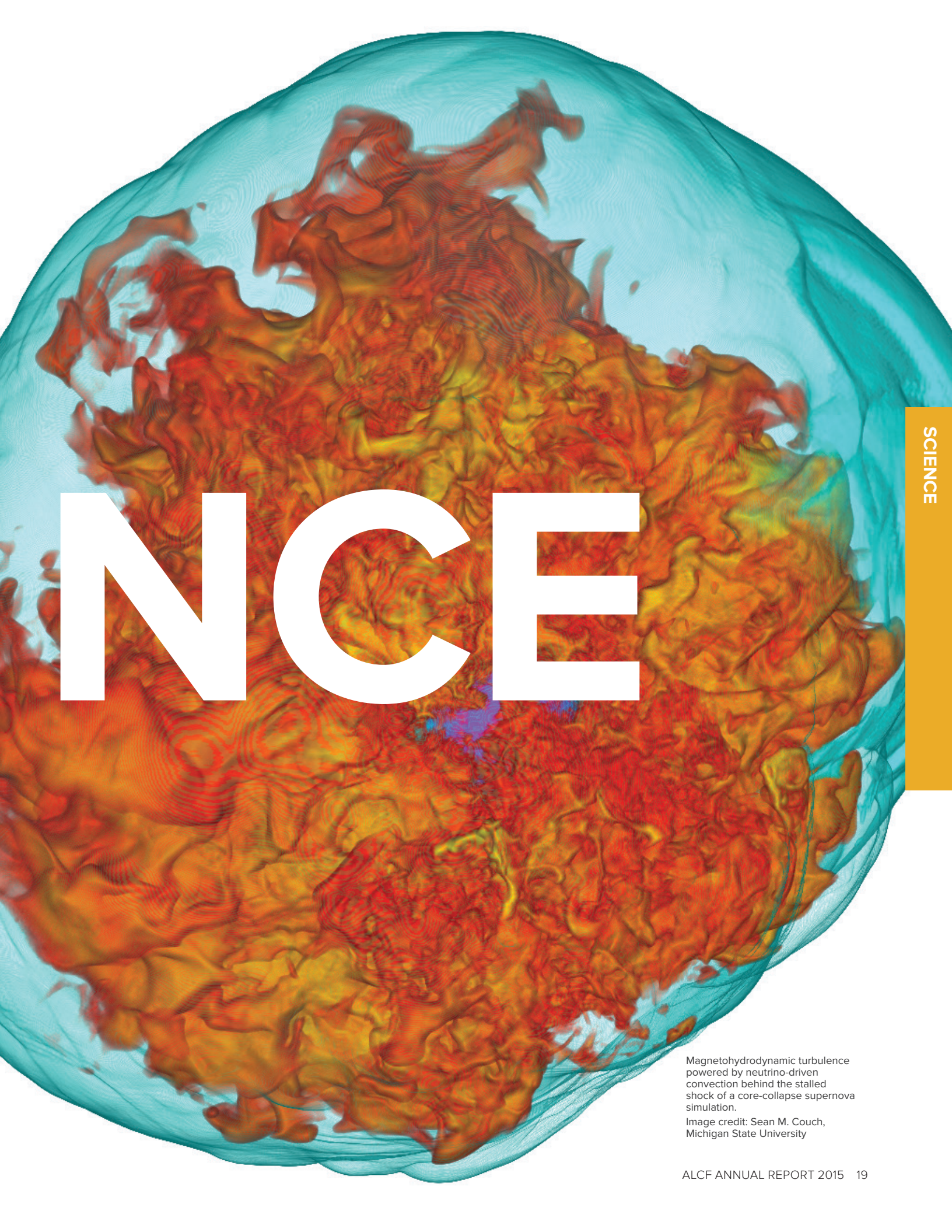
NCE

Magnetohydrodynamic turbulence powered by neutrino-driven convection behind the stalled shock of a core-collapse supernova simulation.
Image credit: Sean M. Couch, Michigan State University
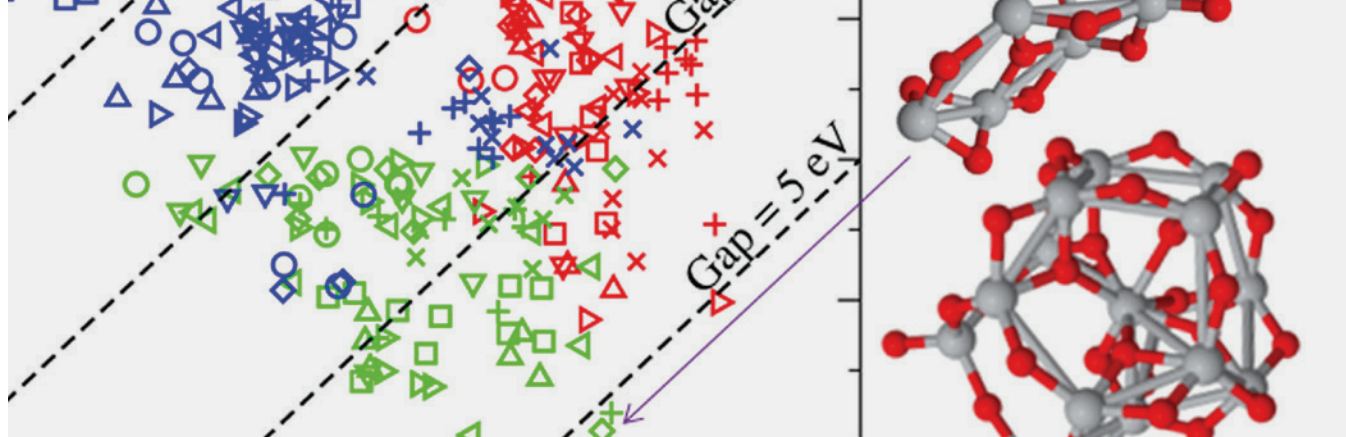
COMPUTATIONAL DESIGN OF
INTERFACES FOR PHOTOVOLTAICS

NOA MAROM

nmarom@tulane.edu
Tulane University

ALCC

120 Million Core-Hours (ALCF: 100M; NERSC: 20M) Chemistry

Image Vertical ionization potential vs. vertical electron affinity for the best 10 structures found by each property-based genetic algorithm for $(TiO_2)_n$ clusters with n=2-20. The loci of constant fundamental gaps are indicated by diagonal lines.

Reproduced from Phys. Rev. B 91, 241115(R) (2015)

The quest for clean, sustainable energy is driving the development of solar energy technologies, such as organic photovoltaics and dye-sensitized, or hybrid, solar cells. One of the main hurdles to reaching maximum efficiency with these devices is the loss of energy within the interfaces between materials. To design more efficient solar cells, scientists need a better understanding of the physical attributes of these functional interfaces at the nanoscale.

APPROACH An international team led by researchers at Tulane University is using Mira to conduct large-scale, first-principles quantum mechanical and molecular dynamics simulations to study these critical interfaces in solar cells. ALCF staff worked with the researchers to optimize the FHI-aims code for Mira, resulting in a 30 percent reduction in runtime for certain calculations. ALCF was also instrumental in helping the team parallelize the GAtor code, a genetic algorithm (GA) designed to find the minimum energy structure of molecular crystals. GAtor interfaces with FHI-aims for first-principles-based geometry optimizations and energy evaluations.

RESULTS For part of the project, the researchers focused on nanostructured interfaces between dye molecules, which absorb sunlight, and titanium dioxide (TiO_2) clusters that help electrons on their way to the electrodes. The researchers found that by nanostructuring the oxide, they could manipulate the energy difference between the oxide and the molecule in order to reduce losses. To optimize the electronic properties, the team implemented GAs to search for $(TiO_2)_n$ (n=2-20) clusters with low energy, a high vertical electron affinity (VEA), and a low vertical ionization potential (VIP). An analysis of the best structures found by these GAs revealed structure-property correlations and enabled the identification of the structural motifs associated with a high VEA and a low VIP (properties that may suggest high reactivity). The researchers demonstrated that the electronic properties of $(TiO_2)_n$ clusters depend more strongly on the presence of these structural motifs than on size, explaining the absence of the expected quantum confinement size trends.

IMPACT This work is advancing first-principles and multiscale simulation techniques to enable researchers to study properties of interfaces that are difficult to resolve experimentally. The theoretical understanding developed in this project will help catalyze new design paradigms for next-generation solar cell technologies.
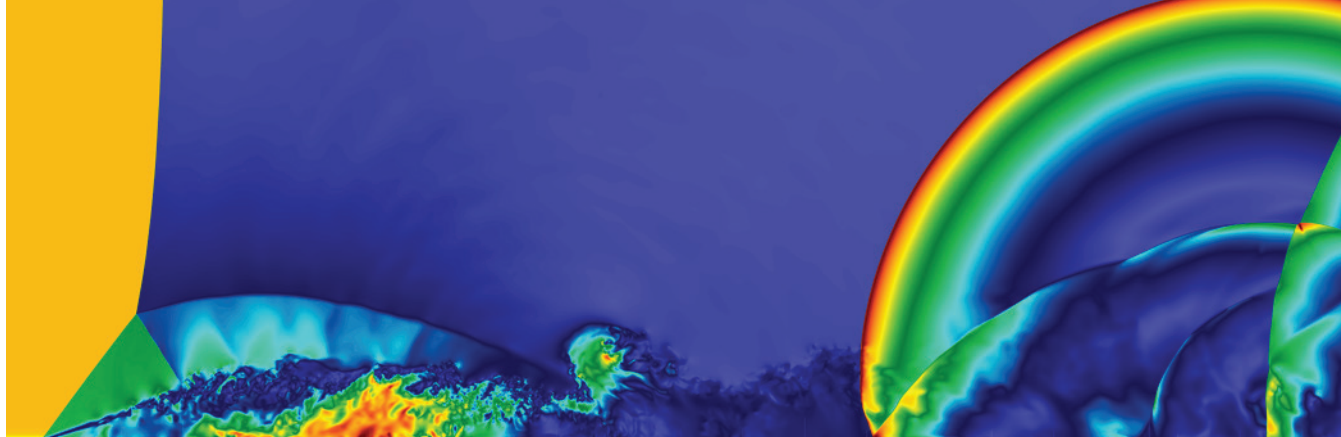
FIRST-PRINCIPLES SIMULATIONS OF
HIGH-SPEED COMBUSTION AND DETONATION

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INCITE

**150 Million Core-Hours
Chemistry**

Image Weak ignition behind a reflected shock in $2H_2+O_2$ mixture at initially atmospheric pressure. The figure shows a 2D distribution of density in the middle of a shock tube with a square cross-section of 5 cm x 5 cm. The end wall of the tube is on the right. The reflected bifurcated shock is on the left and is moving to the left. Weak ignition took place near the end wall approximately 60 microseconds after the shock reflection. The transition of the flame to a detonation happened several microseconds later. Expanding detonation wave is visible on the right.

Image credit: Charles Bacon, Marta García, and Joseph A. Insley, Argonne National Laboratory; Alexei Khokhlov, The University of Chicago; Joanna Austin and Andrew Knisely, University of Illinois at Urbana-Champaign

Detonation waves caused by deflagration-to-detonation transition (DDT) in gaseous mixtures present a significant hazard in the production and delivery of combustible chemicals and fuels. Hydrogen fuel is particularly sensitive to detonation, and DDT hazard is also a potential threat to the safety of certain types of water-cooled nuclear reactors. Because detonation events occur quickly with multiple effects and mechanisms acting concurrently, high-resolution, multidimensional simulations are the most feasible method for investigating the detailed physics of DDT.

APPROACH Researchers from the University of Chicago are using Mira to perform a systematic first-principles study of combustion and detonation phenomena in hydrogen-oxygen mixtures and other reactive gases in various settings. Their study requires using direct numerical simulation (DNS) to explicitly resolve physical processes on spatial scales ranging from meters to microns, as well as attendant shocks, discontinuities, and physical variables. Researchers are performing these simulations with a reactive flow Navier-Stokes high-speed combustion and detonation code, which incorporates detailed physics and chemistry suitable for hydrogen combustion and high-resolution treatment of shock waves. The code also supplies a uniform grid, and static and dynamic adaptive mesh refinement capabilities.

RESULTS The research team has conducted the first 3D reactive flow Navier-Stokes DNS of flame acceleration and DDT in a stoichiometric hydrogen-oxygen mixture at 1 atm initial pressure in a 2.5 cm square pipe with smooth and rough walls. They found wall roughness introduces additional turbulence, which leads to a somewhat faster DDT. It also presents a drastic change in the location of the DDT. In smooth tubes, the DDT was observed ahead of the turbulent flame brush, in a hot gas pre-compressed by the rapidly accelerating flame. However, in the case of rough walls, the team found that the DDT occurs inside the flame brush.

IMPACT This project is using advanced simulations to study the fundamental physics of DDT, providing insights that are not observable in experiments. An improved understanding of the complex mechanisms involved in the detonation of reactive gases will help researchers and engineers to better predict the onset of detonation and develop safety mechanisms for real-world applications.
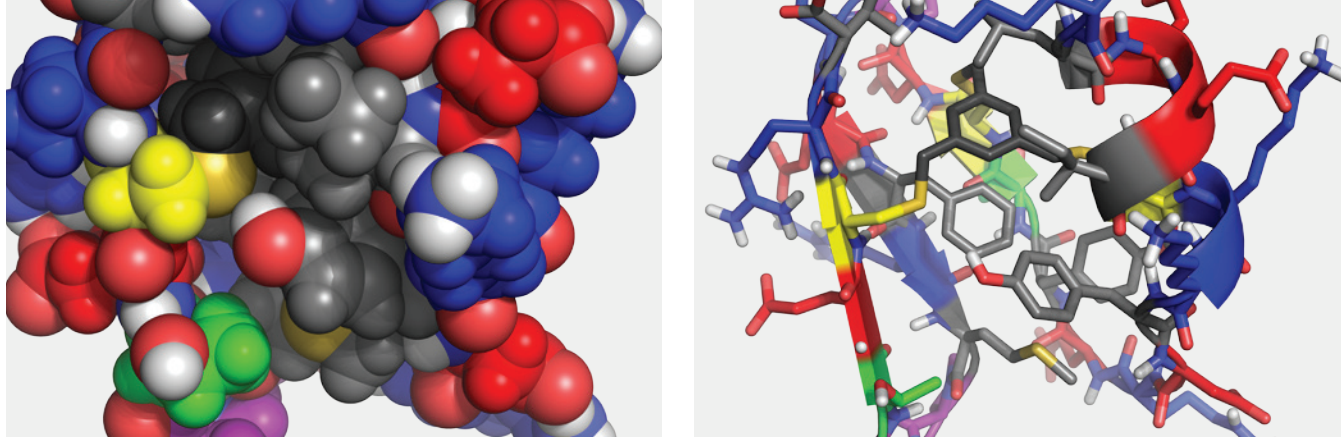
TOWARDS BREAKTHROUGHS IN
PROTEIN STRUCTURE AND CALCULATION AND DESIGN

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University of Washington

INCITE

**80 Million Core-Hours
Chemistry**

Image A designed 29-residue peptide that uses the three-way crosslinker 1,3,5-tris(bromomethyl) benzene (dark gray) to covalently constrain the structure and to form hydrophobic packing interactions with other residues. This molecule is currently being synthesized for experimental examination.

Image credit: Vikram Mulligan, University of Washington

Proteins are large, complex molecules that drive virtually all cellular functions in living organisms. With the emergence of protein structure modeling tools, researchers have the capability to design proteins with targeted applications, such as treating diseases and catalyzing medically and industrially useful reactions. While progress is continually being made to such tools, the ability to sufficiently sample the vast conformational space remains a limiting factor.

APPROACH The Rosetta software suite, developed at the University of Washington's Baker Laboratory, is designed to tackle two difficult computational problems: the prediction of protein structure from amino acid sequences, and the design of new amino acid sequences to yield a desired function. With this INCITE project, researchers are using Mira to enhance Rosetta's ability to sample the vast conformational space and address other emerging challenges in protein structure calculation and design. Their work includes improving the Rosetta energy function and further developing homology model refinement methods. In addition, the researchers are using Mira to design mini-proteins called peptides for a wide range of therapeutic targets, including influenza, Ebola, HIV, and Alzheimer's disease.

RESULTS To enable the peptide design work, the team developed a multistate design approach that allows them to create novel peptides with unique, rigid folds. Their method involves exhaustively enumerating the possible conformations of small peptides with many geometric constraints (e.g., covalent cross-links, terminal peptide bonds). It then uses all of the possible conformational states to search for a sequence that uniquely stabilizes one desired structure and destabilizes all other alternative structures. The search algorithm benefits enormously from Mira's massively parallel architecture, particularly when assigning each conformational state to a separate core.

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

SOI -35°   SOI -24°

Equiv. Ratio [-]
1.00
0.75
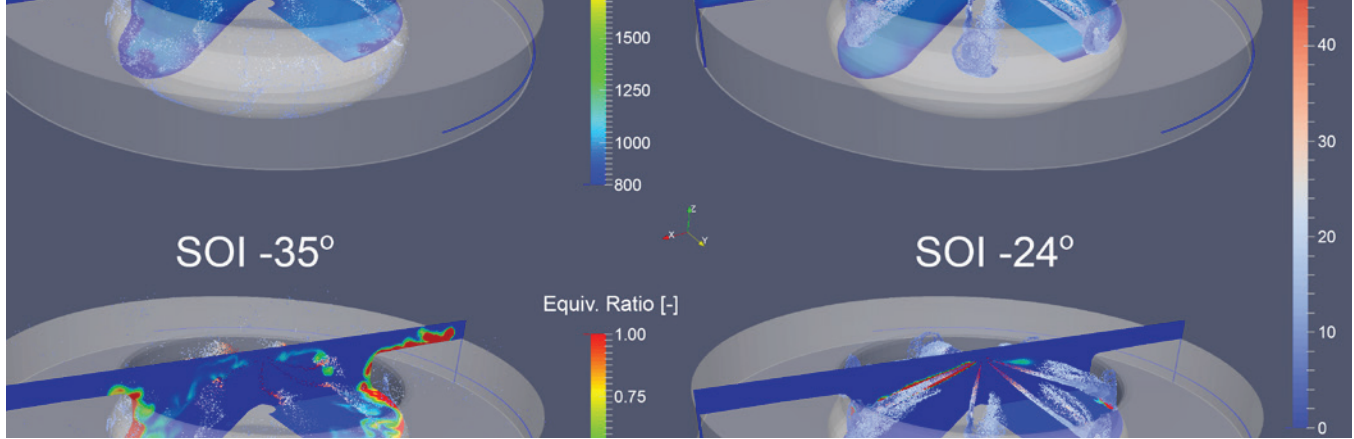
PERFORMANCE IMPROVEMENT
OF CFD CODE CONVERGE
ON BLUE GENE/Q SYSTEMS

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Director's Discretionary

**6 Million Core-Hours
Engineering**

Image This image compares an earlier start of injection (SOI) timing (SOI -35°) to a later SOI timing (SOI -24°). Temperature and equivalence ratio are shown on planes that slice through the domain. Droplets are colored by their radius. With this project, VERIFI researchers demonstrated that in gasoline compression ignition, varying the SOI timing produces significant differences in the reactivity of the fuel mixture, delaying ignition.

Image credit: Stephen Ciatti, Marta García, Kevin Harms, Joseph A. Insley, Janardhan Kodavasal, Christopher Kolodziej, and Sibendu Som, Argonne National Laboratory

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 research team from Argonne National Laboratory is using ALCF resources and expertise to develop more powerful modeling and simulation capabilities that can shed new light on the complex processes taking place inside of internal combustion engines.

APPROACH Researchers from Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI) are working with ALCF staff and Convergent Science Inc. to optimize the CONVERGE code, a commercial computational fluid dynamics (CFD) software tool, for high-performance computing systems. Prior to the team's work at the ALCF, CONVERGE was used to run CFD simulations on up to 50 cores. The ongoing collaborative effort has enabled the code to perform its largest engine simulation to date, running on 8,192 cores on ALCF systems. Their performance optimizations have been focused on the near-ignition portion of the simulation, which is typically the most computationally intensive due to the small timescales associated with calculating chemical kinetics in every CFD cell.

RESULTS The Argonne team modified CONVERGE to use parallel read/write processes, resulting in a more than 100x speedup in writing large data files generated by the software. They also successfully balanced the computational workload evenly across more cores, which led to an 8x improvement in load balancing and a 3.4x improvement in time to solution. The enhancements achieved in this project are machine independent, and are expected to benefit CONVERGE users running the code at scale on any high-performance computing system. These optimizations can also be applied to other CFD software used for engine simulations.

IMPACT This project aims to develop novel engine modeling and simulation capabilities using supercomputers, providing automotive manufacturers with a cost-effective tool to accelerate the development of more energy-efficient engines. Ultimately, these tools have the potential to improve the fuel economy of vehicles, thereby reducing U.S. dependence on foreign oil and reducing carbon emissions.
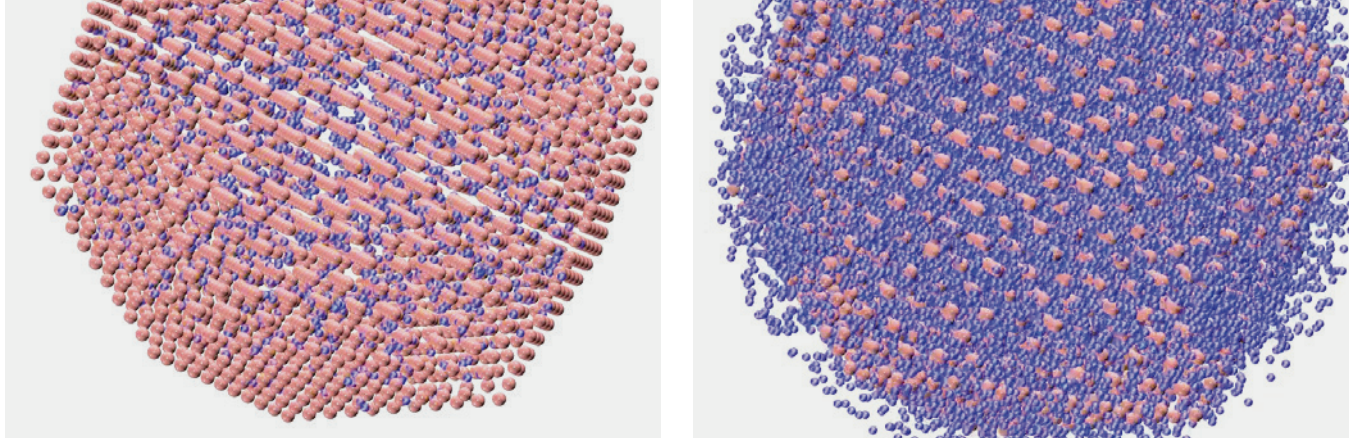
ATOMISTIC COMPUTATIONAL MODEL OF
RADIATION DAMAGE OF NANO-SIZED SYSTEMS IN INTENSE X-RAY PULSES

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Argonne National Laboratory

Director's Discretionary

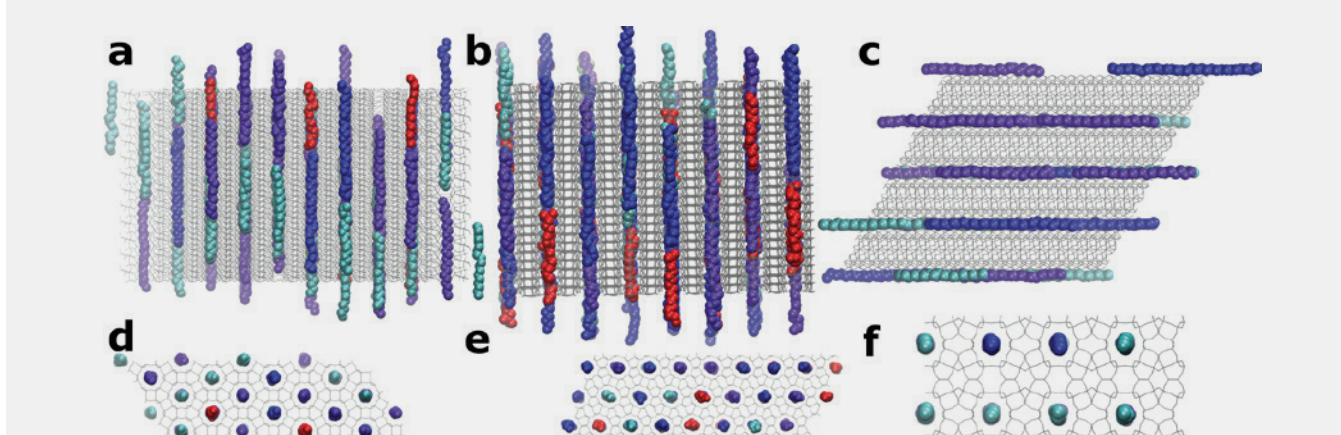**4 Million Core-Hours**
Materials Science

Image Left: A short time after excitation, the initial excitation of argon's 18 electrons (blue spheres) is observed at several places within the 10-shell cluster, comprised of 3,871 argon atoms and 69,678 electrons. Right: At longer times after excitation, many electrons are seen escaping the cluster in all directions.

Image credit: Phay Ho, Christopher Knight, and Linda Young, Argonne National Laboratory

Current x-ray free-electron laser (XFEL) technology allows researchers to fire pulses of a trillion x-ray photons at molecular-sized samples in time scales on the order of femtoseconds. With this tool, researchers are aiming to develop single-particle 3D imaging with atomic resolution, a capability that will enable revolutionary advances in the imaging and study of dynamics of materials. However, with such intense power comes the great challenge of understanding the fundamentals of XFEL-induced radiation damage, which is essential to interpreting the observed measurements and images produced.

APPROACH To understand the nature and amount of damage in nanomaterials at the level of both atoms and electrons, scientists from Argonne's Advanced Photon Source (APS) are using Mira to develop an improved simulation method to model x-ray induced processes in clusters and nanomaterials. The hybrid algorithm uses molecular dynamics (MD) to explicitly track the evolution of all particles in time and a Monte Carlo (MC) algorithm to model the complex quantum mechanical interactions of atoms with an intense x-ray pulse. The team is working closely with ALCF computational scientists to optimize their method within the LAMMPS molecular simulation code.

RESULTS To date, the code has achieved a three-fold speedup by way of improved multi-threaded parallelism in the MC code and force calculations, more efficiently balanced workloads across processors, and optimized I/O. In particular, the time spent in the MC code updating the electronic configurations was reduced from 60 percent to less than 10 percent of the simulation's runtime, making it nearly as fast as normal MD simulations. The code optimizations have allowed the team to explore the ionization of argon nanoparticles as a function of size in various pulse parameters, illuminating the impact of XFEL-induced radiation damage on x-ray diffraction patterns, ion, and electron spectra.

IMPACT This project is providing knowledge and computational tools for modeling interactions of ions and electrons with intense XFEL pulses. This work has potential for significant impacts in the design of single-pulse imaging methods, x-ray optics, and experiments, including those accessible after the APS upgrade.

COMPUTATIONS FOR THE **DEVELOPMENT OF THE NANOPOROUS MATERIALS GENOME**

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Director's Discretionary

**8 Million Core-Hours
Materials Science**

Image Snapshots of representative hydrocarbon configurations inside zeolite frameworks. Views facing the main channel axis (a–c) and along the main channel axis (d–f) are shown for ATO (a,d), MTW (b,e) and PCOD-8113534 (c,f). Zeolite frameworks are depicted as grey lines, and n-octadecane, n-tetracosane, n-triacontane, (2-methyl and 4-methylheptadecane) and 2,2-dimethylhexadecane molecules as cyan, purple, blue, red and green spheres, respectively.

Image credit: Peng Bai and J. Ilja Siepmann, University of Minnesota

In the petrochemical and biofuel industries, aluminosilicate materials called zeolites are used as catalysts and molecular sieves to aid in the processing of fuels and chemical feedstocks. To date, more than 200 types of zeolites have been synthesized and more than 330,000 thermodynamically feasible zeolite structures have been predicted using computational searches. With such a large pool of candidate materials, traditional laboratory methods could take decades to identify the optimal zeolite for a particular application.

APPROACH To help accelerate this process, scientists from the University of Minnesota and Rice University used Mira to demonstrate a predictive theory and modeling tool that can rapidly screen thousands of materials to pinpoint promising candidates for further research and development. ALCF staff helped ensure optimal performance on Mira by guiding the developers of the MCCCS-MN code (Monte Carlo for Complex Chemical Systems) in adding OpenMP support to permit hybrid MPI/OpenMP parallelism, and helping design an MPI-based framework to allow high-throughput calculations capable of using all of Mira's 786,432 cores.

RESULTS The team's computations successfully identified new zeolites for two important applications. One of the zeolites has the ability to purify ethanol from fermentation broths in a single separation step, demonstrating the potential to replace an energy-intensive, multi-step distillation process currently used by industry. To validate the simulation results, the researchers synthesized and tested the promising zeolite, providing experimental data that was in very good agreement with the predictions. For the second application, the team investigated potential zeolite-based catalytic systems for a dewaxing process called hydroisomerization, in which linear long-chain alkanes are transformed into slightly branched alkanes to reduce the pour point and increase the viscosity of lubricant oils and other fuel products. Their simulations identified zeolites with up to 100 times better adsorption capability than current technology used for this process. The research team published results from this project in *Nature Communications*.

IMPACT With the ability to identify optimal zeolites and metal-organic frameworks for particular tasks, this predictive modeling capability has the potential to benefit the production of biofuel and petroleum products, and the development of gas storage and carbon capture devices, while reducing the time and cost of associated laboratory research and development efforts.
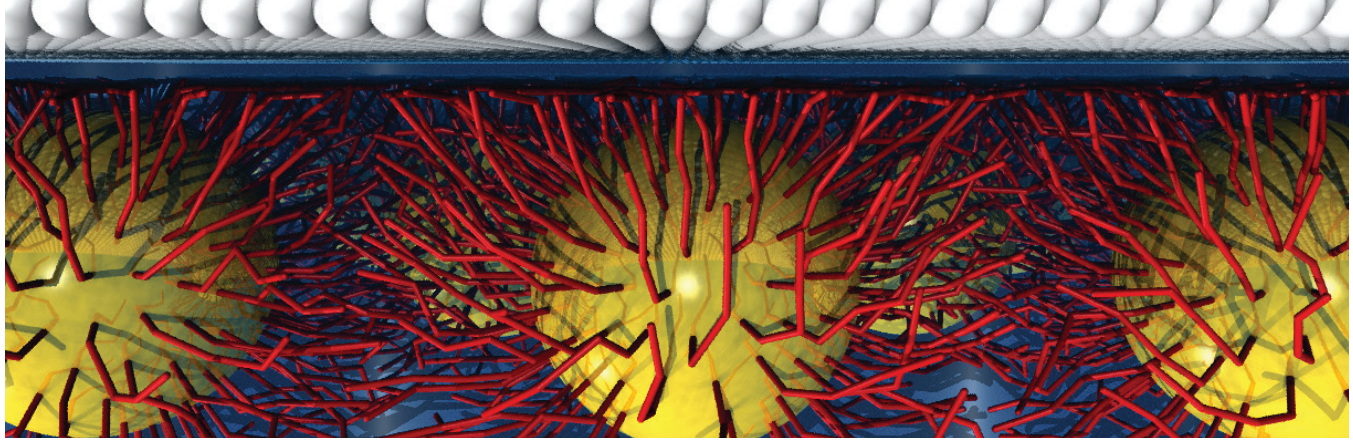
DYNAMICS OF **CONFORMATIONAL TRANSITION IN POLYMER GRAFTED NANOPARTICLES**

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ALCC

**170 Million Core-Hours
Materials Science**

Image An illustration of self-assembled gold (yellow spheres) nanoparticle monolayers on supporting interfaces (white spheres) showing preferential asymmetry in ligand (red sticks) coverage.

Image credit: Joseph A. Insley and Subramanian Sankaranarayanan, Argonne National Laboratory

Nature is capable of constructing curved membranes to form complex cellular structures in biological systems. Scientists are interested in tailoring this naturally occurring process to advance the design of membranes with tunable electrical, magnetic, and mechanical properties for applications, such as sensors.

APPROACH In a combined experimental/modeling investigation, researchers from Argonne National Laboratory, the University of Chicago, and the University of Missouri discovered a practical route to creating folded nanoparticle membranes as a result of producing molecular asymmetries on their surface. By tuning the amount of ligand molecule coverage on gold nanoparticles, the researchers identified a small but significant asymmetry in self-assembled nanoparticle monolayers caused by the heterogeneous environment when formed on water droplets. They found that the difference in ligand coverage was the controlling factor for subsequent bending towards the water-facing side of the membrane when exposed to electron beams. Using Mira, the team performed large-scale molecular dynamics simulations to corroborate the extensive experimental characterization of these nanoparticle membranes and the bending process.

RESULTS As part of the computational work, the team developed an atomistically informed coarse-grained MARTINI model for the nanoparticles wherein small groups of similar molecules are modeled as a single effective particle. Researchers then carried out coarse-grained simulations to model the long-time dynamics of nanoparticle membrane self-assembly at the air-water interface. In large-scale simulations spanning 1–2 microseconds using as many as eight racks of Mira, they identified a strong correlation between ligand mobility on the nanoparticles and an asymmetric coverage at the air-water interface revealing microscopic details of the nanoparticle self-assembly process. Similar to experiments, the researchers systematically varied the ligand coverage of nanoparticles to understand the microscopic mechanism responsible for the asymmetry. This effort resulted in a magnitude of asymmetry that was in agreement with experimental observations. The team's results were published in *Nature Materials*.

IMPACT This work demonstrates that nanoscale differences in self-assembled structures can lead to changes in macroscopic physical properties. Tuning the degree of this asymmetry (and thus bending) in response to environmental conditions is key to designing membranes with tunable properties. The results provide an important step forward for creating nanoparticle assemblies tailored for specific applications, such as mechanical, chemical, and biological sensors.
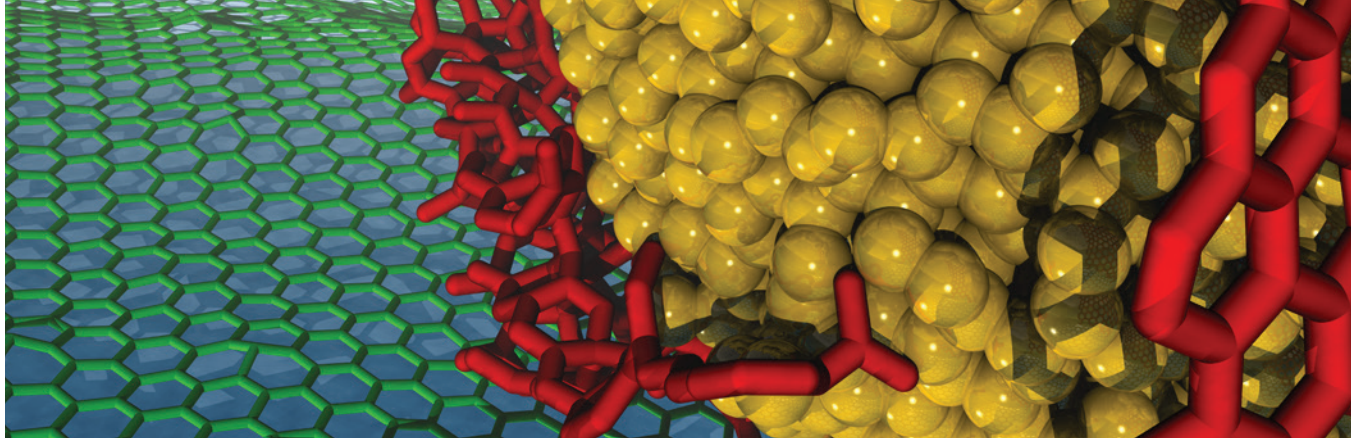
REACTIVE MD SIMULATIONS OF
ELECTROCHEMICAL OXIDE INTERFACES AT MESOSCALE

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INCITE

**40 Million Core-Hours
Materials Science**

Image This visualization depicts a phenomenon called superlubricity, a property in which friction drops to near zero. The team's simulations revealed that this condition originates at the nanoscale when graphene atoms self-assemble into nanoscrolls that reduce contact area to help eliminate friction.

Image credit: Sanket Deshmukh, Joseph A. Insley, and Subramanian Sankaranarayanan, Argonne National Laboratory

Superlubricity—a state in which friction essentially disappears—is a highly desirable property for automobiles, wind turbines, and countless other mechanical assemblies that lose efficiency to friction. Argonne scientists recently made strides toward superlubricity with the development of a lubricant material consisting of graphene and diamond-like carbon. In experimental tests, the material was showing signs of superlubricity, but its friction levels were fluctuating up and down for no apparent reason.

APPROACH To shed light on the mysterious behavior, Argonne computational scientists used Mira to replicate the experiments with large-scale molecular dynamics simulations aimed at understanding the underlying mechanisms of superlubricity at an atomistic level. ALCF staff helped to enable the computationally demanding simulations by optimizing the LAMMPS code and its ReaxFF module. The optimization work included adding OpenMP threading, replacing MPI point-to-point communication with MPI collectives in key algorithms, and leveraging MPI I/O. Altogether, these enhancements enabled the code to perform twice as fast as before.

RESULTS The simulations revealed a completely new mechanism for superlubricity. When the graphene and diamond-like carbon slid against each other, the graphene rolled up to form hollow cylindrical "nanoscrolls" that helped to practically eliminate friction. The researchers determined that the fluctuating friction levels were caused by the fact that the nanoscrolls themselves were not stable. By incorporating nanodiamond particles into the simulations, the team was able to stabilize the nanoscrolls, which resulted in sustained superlubricity. The simulation results informed the design of a hybrid material that demonstrated superlubricity in laboratory tests as well. Although the material does not work in the presence of water, the discovery shows great potential for applications in dry environments. Results from this project were published in *Science*.

IMPACT This work led to the development of a material that exhibited superlubricity at the macroscale for the first time. The material could potentially be used for applications in dry environments, such as computer hard drives, wind turbine gears, and mechanical rotating seals for microelectromechanical and nanoelectromechanical systems. In addition, the knowledge gained from this study is expected to spur future efforts to develop materials capable of superlubricity for a wide range of mechanical applications.
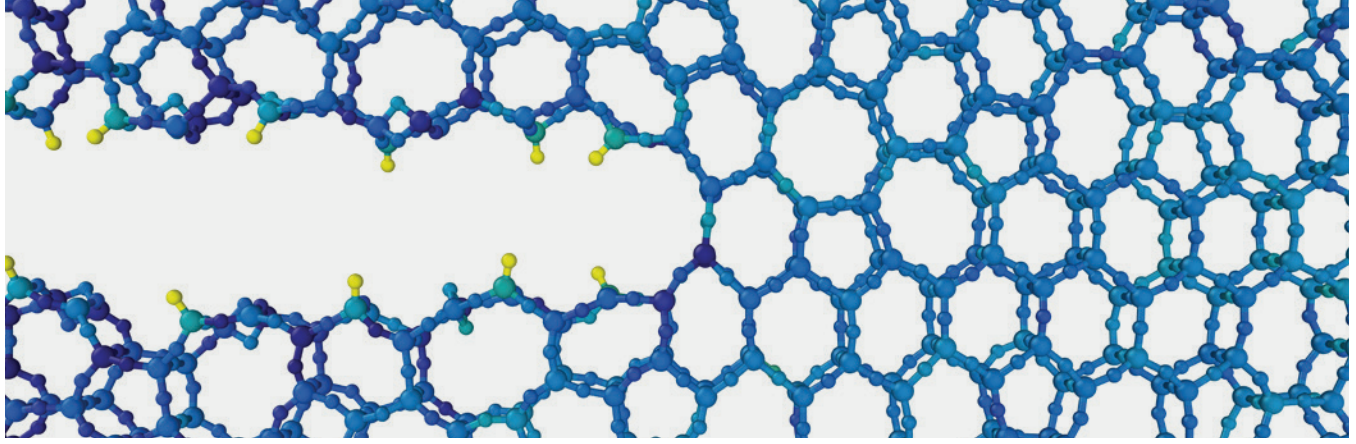
SiO$_2$ FRACTURE: CHEMOMECHANICS
WITH A MACHINE-LEARNING
HYBRID QM/MM SCHEME

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University of Warwick

INCITE

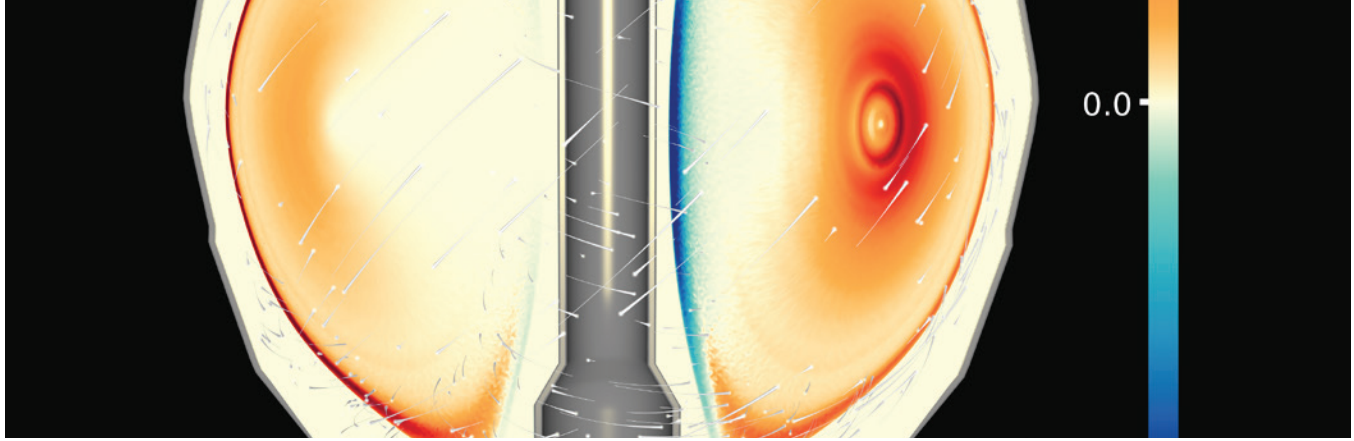**125 Million Core-Hours
Materials Science**

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

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

Fracturing minerals requires a tremendous amount of energy. In mining, the energy spent fracturing represents almost 85 percent of such activity. The World Business Council estimates that mining is responsible for nearly 5 percent of total human energy consumption, and annually releases millions of tons of carbon dioxide. Understanding the physical process of grinding and crushing minerals under different environments has a technological and scientific relevance to reduce the ecological footprint of mining.

APPROACH A collaborative team from the University of Warwick, King's College London, the University of Basel, and Argonne National Laboratory is using Mira to improve the techniques required to understand the intricate mechanisms of fracturing materials, and to overcome the challenges of simulating large materials and complex physical processes at atomic resolution. The team is employing a quantum mechanical/molecular mechanical (QM/MM) approach coupled with a Machine Learning on-the-Fly (MLOTF) method, which is of particular interest since it enables the systematic study of large systems with QM precision for the first time. ALCF staff helped the project to move forward by porting the CP2K electronic structure code and enabling an optimized version of the linear algebra library ELPA for large QM simulations.

RESULTS The team's work is advancing the techniques required to understand the intricate mechanisms of fracturing materials, and is helping to overcome the challenges of simulating large materials and complex physical processes at atomic resolution. The MLOTF scheme efficiently combines classical and quantum mechanics to study bond breaking in amorphous systems. The researchers have demonstrated that MLOTF works on the fracture of real 3D materials such as silicon and silica, common components in rocks. In practical tests, MLOTF has shown a speedup of up to 10^3 compared to carrying out QM calculations at every time step.

IMPACT This research has implications for the manufacture of silica-based products resistant to fracture, and could significantly reduce energy and cost expenditures associated with mineral ore processing. The methodology used has potential future application in the study of a wide variety of materials and processes.

HIGH-FIDELITY SIMULATION OF
TOKAMAK EDGE PLASMA TRANSPORT

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INCITE

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

Image Developed from simulations on Mira, this image shows trapped (left cross-section) and passing (right cross-section) electrons carried in the bootstrap current of a tokamak, which is in contrast to the previous understanding that the bootstrap current is carried by passing particles only. Based on a series of high-resolution simulations of bootstrap current in present-day tokamak geometries, researchers have modified a well-known formula that calculates the value of bootstrap current in order to improve the prediction of fusion efficiency in tokamak reactors.

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

With the potential to produce a clean and virtually inexhaustible energy supply, fusion power could be a global solution to future energy demand. But many difficult scientific problems first must be understood and overcome before a functional fusion power plant can be realized. One of the biggest obstacles to building a magnetically confined fusion energy system, such as ITER, is confining the plasma within a practical amount of space. A well-confined edge plasma forms a steep pedestal and puts the fusion plasma into a high-confinement mode, which allows an efficient fusion burn in the plasma core.

APPROACH Researchers from the Princeton Plasma Physics Laboratory are using XGCa, the latest iteration of the XGC gyrokinetic code, to gain an understanding of the underlying plasma physics that govern edge plasma confinement in fusion reactors. With help from ALCF staff, the researchers were able to run simulations with XGCa on more than 260,000 cores with excellent scalability, allowing the team to accurately evaluate a strong self-generated electrical current, called "bootstrap current," that runs through the plasma. This current helps enable better confinement of the edge plasma, and therefore higher fusion efficiency.

RESULTS The team's simulations revealed electron behaviors related to bootstrap current that are not accurately predicted for present-day tokamak geometry by the Sauter formula, which is used to calculate values for the bootstrap current. Two types of electrons characterize bootstrap current: passing and trapped. Based on tokamak geometries with large aspect ratios, physicists have understood for decades that passing electrons in the core plasma are primarily responsible for carrying the bootstrap current. However, with more detailed simulations of trapped and passing electrons of the edge plasma, the INCITE researchers observed that trapped electrons can take on the responsibility of carrying bootstrap current at the edge where there are fewer passing electrons. Numerous simulations for different geometric and plasma conditions led to a new unified analytical formula that can describe the edge current, as well as the core current.

IMPACT This new analytical formula is expected to be widely used by international fusion researchers studying edge plasma physics. This will enable the fusion research community to better understand and predict edge plasma behavior, and to ensure highly efficient tokamak performance and more economical ITER operation.
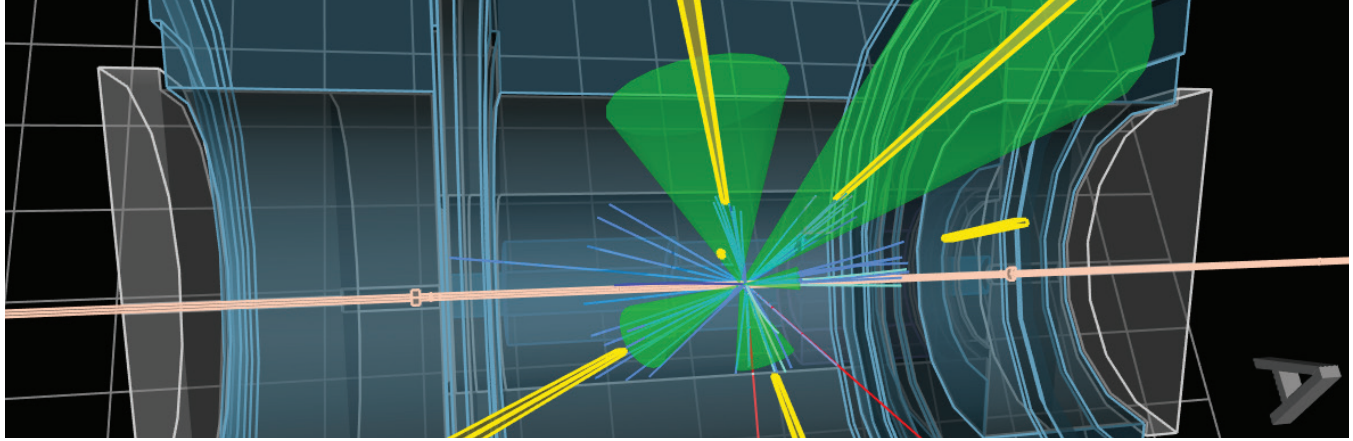
SIMULATION OF **LARGE HADRON COLLIDER EVENTS USING LEADERSHIP COMPUTING**

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Argonne National Laboratory

ALCC

52 Million Core-Hours (ALCF: 50M; NERSC: 2M) Physics

Image A visualization of a simulated collision event in the ATLAS detector. This simulation, containing a Z boson and five hadronic jets, is an example of an event that is too complex to be simulated in bulk using ordinary PC-based computing grids.

Image credit: Taylor Childers, Argonne National Laboratory

Scientists from across the world use CERN's Large Hadron Collider (LHC) to explore the behavior of matter, energy, space, and time at the smallest scales ever probed. Computer simulations are key to helping them understand the response of the LHC detectors in particle collisions at the facility. Differences between observations and simulation data can lead to discoveries of new physics. However, some LHC events are so complex that it would take weeks to complete the calculations on LHC's computing grid, a system of 100,000 PC-like computers distributed all over the world. In addition, the LHC's computing needs are expected to grow by at least a factor of 10 over the next several years.

APPROACH Argonne researchers are using Mira to explore the potential of supercomputers to enable future discoveries at LHC. In particular, they are focusing on collision events in the ATLAS experiment that are difficult to simulate with traditional computing resources. ALCF staff worked closely with Argonne physicists to transform ALPGEN, a Monte Carlo-based application that generates events in hadronic collisions, from a single-threaded simulation code into massively multi-threaded code that could run efficiently on Mira. By improving the code's I/O performance and reducing its memory usage, they were able to scale ALPGEN to run on the full Mira system and help the code perform 23 times faster than it initially did.

RESULTS The code optimization work has enabled the team to routinely simulate millions of LHC collision events in parallel. The improved throughput allowed them to complete two years' worth of ALPGEN simulations in a matter of weeks, freeing the LHC computing grid to run other jobs. Throughout the course of the ALCC project, the team's simulations equated to about 9 percent of the annual computing done by the ATLAS experiment. Ultimately, this effort is helping to accelerate the science that depends on these simulations.

IMPACT With this project, Argonne researchers are showing that supercomputers like Mira can help drive future LHC discoveries. Running particle collision simulations on DOE leadership computing resources provides three key benefits to LHC experiments: increasing the amount of simulated data that can be produced; simulating more complex and realistic events than are currently possible; and helping to evolve LHC's substantial code base for current and future supercomputing platforms.
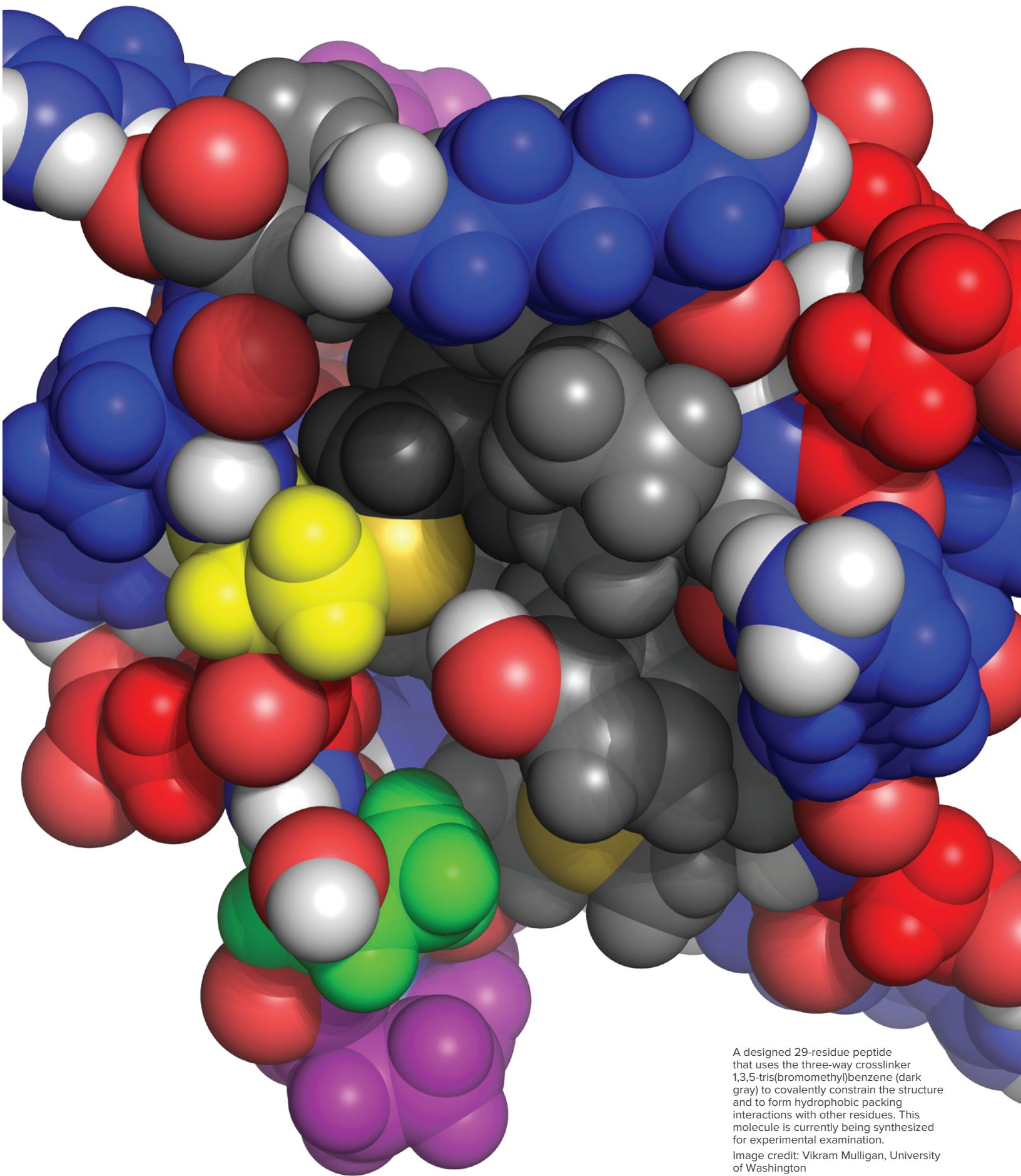
A designed 29-residue peptide that uses the three-way crosslinker 1,3,5-tris(bromomethyl)benzene (dark gray) to covalently constrain the structure and to form hydrophobic packing interactions with other residues. This molecule is currently being synthesized for experimental examination.

Image credit: Vikram Mulligan, University of Washington

PEO

With a shared passion for research and innovation, the ALCF's talented and diverse staff help make the facility one of the world's premier centers for computational science and engineering.

PLE

77

STAFF
MEMBERS

13

POSTDOCTORAL
RESEARCHERS

24

SUMMER
STUDENTS

ALCF EXPERTISE

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

Catalysts

Catalysts are computational scientists who work directly with project teams to maximize and accelerate their research efforts. With multidisciplinary domain expertise, a deep knowledge of the ALCF computing environment, and experience with programming methods and community codes, the team helps users surmount any obstacles they may encounter using ALCF computing resources. This includes collaborating with colleagues from other ALCF teams to resolve issues when additional expertise is required.

Data Analytics and Visualization

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

Operations

Operations ensures that system hardware and software work reliably and optimally; system tools are matched to the unique system architectures and scale of ALCF resources; the entire system software stack works smoothly together; and I/O performance issues, bug fixes, and requests for system software are addressed.

Performance Engineers

Performance Engineers help users achieve optimal performance on ALCF resources by working with them to port, tune, and parallelize scientific applications and other software on current and emerging systems. The team also helps drive the future of high-performance computing and data-intensive computing through research and development of performance models and scalable algorithms, and the development of standards for key areas, such as benchmarks, compilers, and programming models.

User Experience

User Experience coordinates communications, support, and outreach for the ALCF. The communications team stewards ALCF user stories and ensures that the facility provides relevant and accurate information to users, DOE, and the public at large. The support team manages the workflows for user accounts and projects, and assists users with support requests related to their ALCF projects. Outreach focuses on organizing training efforts and user-centered events for the ALCF.

ALCF WELCOMES TWO NEW DIRECTORS

The ALCF filled two important leadership positions in 2015.

KATHERINE RILEY
Director of Science

The ALCF is familiar territory for Katherine as she was one of the facility's first hires in 2007. In her current role as Director of Science, she leads scientific strategy for the ALCF, ensuring the facility delivers leading-edge computational capabilities and expertise that help advance fundamental discovery and understanding in a broad range of scientific and engineering disciplines.

Katherine has spent her career focused on scientific application architecture and how it impacts performance, scalability, and extensibility. She previously served as a principal scientific applications engineer and manager of the ALCF catalyst team, a group of computational scientists who work directly with users to help them maximize their time on ALCF systems and achieve their research goals. Katherine has also been a key contributor to the strategic vision of the facility, assisting with the design and development of ALCF supercomputers by helping to identify the scientific requirements for new systems.

Prior to joining the ALCF, she served as scientific applications engineer in the Mathematics and Computer Science Division at Argonne and as a senior scientific programmer at the University of Chicago.

> **Katherine cultivates and guides teams of scientists and engineers to use one of the most powerful supercomputers in the world dedicated to open science.**

MARK FAHEY

Director of Operations

As ALCF Director of Operations, Mark is responsible for the day-to-day operations of the facility's computing systems, including Mira, a 10-petaflops IBM Blue Gene/Q supercomputer. He oversees a team with extensive expertise in all aspects of high-performance computing hardware and software, including advanced integration, system and network administration, infrastructure, and storage.

While Mark is new to the ALCF, he is no stranger to high-performance computing in the national laboratory environment. Prior to coming to Argonne, he was the deputy director of the National Institute for Computational Sciences, a National Science Foundation-funded computing center co-located at the University of Tennessee and Oak Ridge National Laboratory. Mark was also senior research staff in the Scientific Computing Group at the Oak Ridge Leadership Computing Facility for over 13 years.

In addition, Mark is a co-developer of the XALT and ALTD library tracking infrastructures, which are in use at various high-performance computing centers around the world.

Mark coordinates and manages the facility's operational activities, ensuring that ALCF systems meet performance metrics as well as users' science needs.

STAFF SPOTLIGHTS

Savannah (Xiao) French
UX Developer

While pursing her degrees in actuarial science and computer science at North Central College, Savannah landed an internship as a research aide at the ALCF. Her first task was to design and build an interactive website graphic that displayed real-time information about the jobs running on Mira. In 2015, Savannah was hired as a full-time developer on the user experience team. In addition to helping maintain the ALCF website, she designs and develops research and event websites for strategic initiatives. Savannah was also a key part of the team that executed the ALCF's annual user survey, participating in every step of the process from reviewing survey questions and following up with users to analyzing the final results. The team's efforts resulted in the survey's highest response rate ever.

Marta García
Computational Scientist

As a member of the catalyst team, Marta works closely with science teams to maximize their use of ALCF computing resources. Her expertise in computational fluid dynamics has made her a key collaborator on several projects, including work to develop advanced engine modeling and simulation capabilities. In 2015, Marta played an important role in helping Argonne build its future R&D programs and capabilities, chairing the Director's Review Committee for Competitive Grants for the Laboratory Directed Research and Development (LDRD) Program. She was also one of four Argonne researchers featured in the "Catch a Rising Science Star" public lecture, which showcased some of Argonne's best and brightest young scientists. In 2016, Marta will take the reins from former ALCF Director of Science Paul Messina as the program manager of the Argonne Training Program on Extreme-Scale Computing.

Christopher Knight
Computational Scientist

Chris served as a guest lecturer at Harvard University this fall, leading six sessions as part of a graduate-level course on extreme-scale computing. The hands-on lessons, which included running jobs on Mira, helped the students (most of whom did not have a background in science) understand how supercomputers can be used to address real-world problems, such as designing better batteries. At the ALCF, Chris's recent work with a University of Minnesota team resulted in a *Nature Communications* paper that discussed their promising results with a predictive modeling tool for identifying optimal zeolites. He is now co-PI for the team's ALCC project focused on modeling functional nanoporous materials. Chris is also working closely with an Argonne/University of Chicago team investigating materials for energy conversion and storage, serving as co-PI of an ALCC award and a collaborator for their Theta ESP project.

Scott Parker
Performance Engineer

As a performance engineer, Scott helps the facility and its users get the most out of Mira. In addition to porting and tuning scientific applications for the massively parallel supercomputer, he develops software tools, such as the recently deployed AutoPerf library, that are aimed at achieving better performance on ALCF systems. Launched this fall, AutoPerf collects performance data during simulation runs to give Scott and his colleagues a better understanding of application requirements. Scott is also a key contributor to the facility's preparations for its future supercomputers. He has begun analyzing benchmark codes running on simulator software and early hardware to gather performance information that will ultimately help users adapt and tune their codes for the next-generation systems. His efforts have included visits to Intel's Hillsboro, Oregon campus to work directly with Intel employees and computing resources.

Skip Reddy
HPC Infrastructure Lead

Skip specializes in high-performance computing environments, but he's also making a significant impact on the workplace environment at Argonne. In 2015, he co-founded Spectrum, an employee resource group dedicated to building awareness and providing resources for the lesbian, gay, bisexual, transgender, queer, and allies (LGBTQA+) community. As a board member of Spectrum, Skip is helping to lead the group in its efforts to promote a welcoming and inclusive laboratory community, advance LGBTQA+ friendly policies and benefits, and participate in outreach and talent recruitment activities. At the ALCF, Skip oversees the team responsible for the facility's supporting systems environments. Among their notable achievements in 2015, Skip's team installed and deployed Cooley, the ALCF's new visualization and data analysis cluster, and upgraded the NetApp filers, which provide storage to management systems and business intelligence, and crucially, allow Mira to boot full-system jobs rapidly and reliably.

Silvio Rizzi
Postdoctoral Researcher

As a PhD student at the University of Illinois at Chicago, Silvio's work focused on developing immersive simulation tools to allow neurosurgeons to practice surgical procedures in realistic virtual environments. Since joining the ALCF in 2013, Silvio has put his experience with 3D models and scientific visualization to work, but in a much different context and on a much larger scale. His research now focuses on novel algorithms for large-scale visualization and analysis. As part of the visualization team, he interacts with researchers from a variety of disciplines to help them better understand enormous numerical datasets from some of the largest simulations performed to date. In 2015, Silvio developed a particle-based method for the vl3 visualization framework, which helped a team of Argonne scientists visualize a simulated universe with data from their massive cosmological simulation.

STAFF SPOTLIGHTS

TECH

ALCF researchers are helping to develop the technologies needed to drive continued improvements in supercomputing performance.

ENABLING SCIENCE THROUGH HPC TECHNOLOGY

ALCF researchers are developing software tools and approaches that are helping scientific applications run more efficiently on its leadership-class systems.
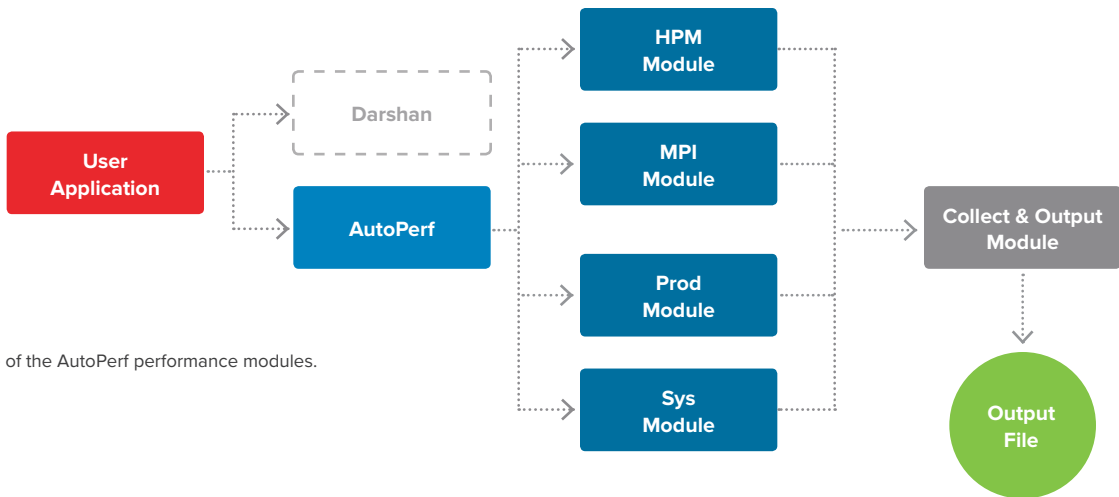
AutoPerf

Launched in 2015, AutoPerf is an ALCF-developed library that automatically collects performance information for applications running on ALCF systems. The tool records data from simulations and saves it into files for analysis when the job is completed. Output includes MPI usage and performance information that indicates which MPI routines were called, how many times each routine was called, the time spent in each routine, the number of bytes sent or received (if applicable), and data from the systems' hardware performance counters. This information will help ALCF staff better understand the requirements of applications and how to optimize their performance.

Compiler and Library Tracking

The ALCF deployed two software tools in 2015 to track the compilers and libraries being used on its systems. The first stage in the library-tracking process is a component called Trackdeps, which records paths to all inputs to the build process that contribute to the final output, including compiler identity, header files, Fortran module files, and libraries. Tracklib, the second stage in the library-tracking process, is a set of tools used to examine programs as they run on Mira, producing the data necessary to match the job's accounting information with the data collected by Trackdeps. With these tools in place, staff can determine how various libraries and compilers are being used at the facility, providing knowledge that helps inform support and research priorities for the ALCF and DOE.

Darshan

ALCF researchers are collaborating with staff from Argonne's Mathematics and Computer Science Division on the continued development of Darshan, a scalable HPC I/O instrumentation library designed to capture an accurate picture of application I/O behavior. This tool records statistics such as the number of files opened, time spent performing I/O, and the amount of data accessed by an application. Darshan's lightweight design makes it suitable for full-time deployment for workload characterization of large systems. The information revealed by Darshan enables researchers to investigate and tune the I/O behavior of complex HPC applications, while also helping the storage research community to develop strategies and approaches to better serve the needs of scientific computing. Darshan was originally developed on the IBM Blue Gene series of computers at the ALCF, but it is portable across a wide variety of platforms and is now deployed at multiple DOE computing facilities including NERSC, OLCF, and Lawrence Livermore National Laboratory.

The structure of the AutoPerf performance modules.

Cobalt

Developed at Argonne, Cobalt is the ALCF's job scheduler and resource manager. This tool gives the facility great flexibility in executing its scheduling policies, accommodates diverse workloads, and supports important features (e.g., alternate kernel support) that are either not supported or poorly supported by other schedulers and resource managers. The ALCF continues to develop and improve Cobalt to meet future resource scheduling needs. In 2015, ALCF researchers began preparing Cobalt to support its next-generation systems, Theta and Aurora, when they are deployed. The Cobalt development team also implemented a draining and backfilling scheme for cluster systems, like Cooley, which improves utilization of the resource and prevents excessive delays in the start of jobs with larger node counts.

GLEAN

ALCF researchers are developing an open source software tool called GLEAN to help users optimize data movement between the compute, analysis, and storage resources of HPC systems. GLEAN improves I/O performance by exploiting the network topology for collective I/O, leveraging data semantics of applications, and incorporating asynchronous data staging. GLEAN can also be used to perform *in-situ* analysis during large-scale simulation runs, which allows researchers to analyze data in real time. Algorithms and components of GLEAN are being used by projects running on ALCF systems, and are being integrated with the IBM system software stack to benefit users of IBM Blue Gene/Q systems.

Optimal Scheduling of *In-Situ* Analysis

With *in-situ* analysis, researchers can perform real-time data analysis and visualization during large-scale simulation runs. To help facilitate this capability, ALCF researchers are investigating the challenge of scheduling the analyses with the simulation. The team used a mixed-integer linear program to maximize the number of online analyses subject to resource constraints, such as I/O bandwidth, network bandwidth, rate of computation, and available memory. Using Mira, they performed case studies with the LAMMPS and FLASH codes that demonstrated the effectiveness of their approach. The results were presented at SC15. The team plans to extend this work by optimally scheduling the analyses computations on different resources.

NEW SYSTEMS PROVIDE ADVANCED CAPABILITIES

Leading-edge computing technologies are intrinsic to the ALCF. The facility is continually developing and deploying resources that support forefront computational research.
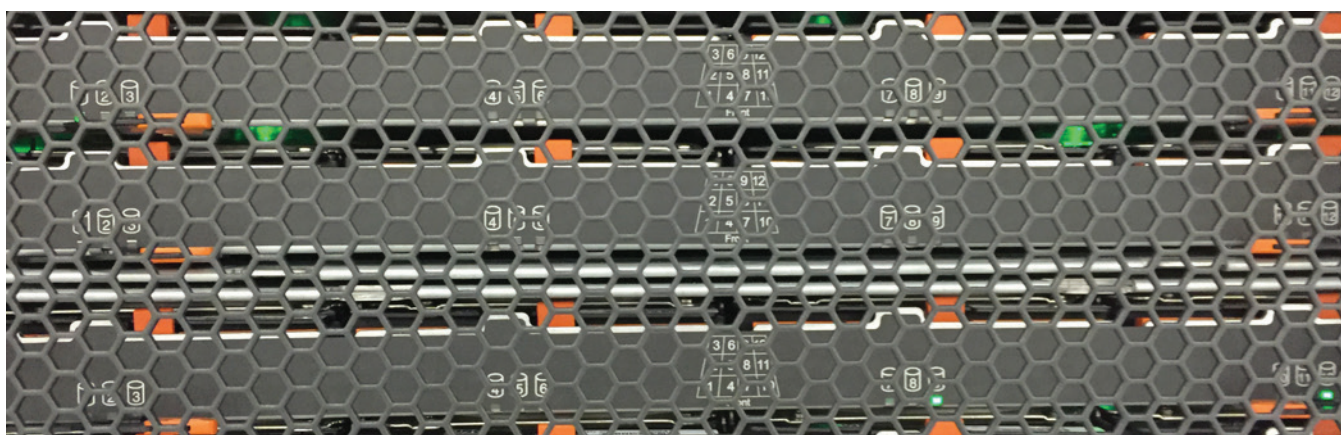
Cooley

In June, the ALCF launched Cooley, a new visualization and analysis cluster with nearly eight times the memory capacity of the facility's previous system, Tukey. This significant memory boost, along with Cooley's state-of-the-art hardware, is helping ALCF users to better analyze and explore the massive datasets that result from their simulations on Mira. Some of the new and improved capabilities enabled by Cooley include: *in-situ* analysis, volume-rendered visualizations, meshing complex geometries, and uncertainty quantification analysis.

Storage Upgrade

The ALCF is in the midst of a storage infrastructure upgrade aimed at reducing the amount of time users have to spend on data management and I/O efforts. In 2014, the operations team added a second IBM General Parallel File System (GPFS) to compliment its primary GPFS. This year, they continued work on a burst buffer-like storage cache that is being developed to provide users with much faster I/O rates for running jobs. The team is also working on a service to automatically archive data to long-term storage. In addition, they tripled the facility's archival storage capacity by replacing its LTO4 tape drives with LTO6 tape drives.

Petrel

Researchers from ALCF and Globus are collaborating to develop Petrel, a pilot data service that allows researchers to store and share large-scale datasets with collaborators without the burden of local account management. Petrel leverages the ALCF's storage and infrastructure and Globus's transfer and sharing services to provide a mechanism to store large research data, move data in and out of the system, and make subsets of the data available to collaborators. Petrel has been deployed for researchers at Argonne's Advanced Photon Source and will be expanded to other ALCF users in the near future.

ALCF COMPUTING RESOURCES

MIRA

Mira, the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer, opens the door for scientists to analyze data more efficiently, design products more quickly, and address some of society's biggest problems in ways that would otherwise be impossible. The system is capable of carrying out 10 quadrillion calculations per second. Mira is also among the most energy-efficient supercomputers, saving considerable energy through innovative chip designs and a unique water-cooling system.

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

CETUS

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

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

VESTA

As the ALCF's test and development platform, Vesta serves as a launching pad for researchers preparing to use Mira. Vesta has the same architecture as Mira, but on a much smaller scale.

- 2 racks
- 2,048 nodes
- 32 TB RAM
- 5D torus interconnect
- 32 I/O nodes
- Peak performance of 419 teraflops

Susan Coghlan and Eric Pershey of ALCF discuss computing hardware in the facility's machine room.

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

COOLEY

Cooley is the ALCF's analysis and visualization cluster. Equipped with graphics processing units (GPUs), Cooley converts computational data from Mira into high-resolution visual representations. The resulting images and videos help users to better analyze and understand the data generated by Mira. Cooley can also be used for statistical analysis, helping to pinpoint trends in the simulation data. Additionally, the system is capable of preprocessing efforts, such as meshing, to assist users preparing for Mira simulations. Cooley shares file systems with Mira, enabling direct access to Mira-generated results.

Each Cooley node has:

- 2 2.4 GHz Intel Haswell E5-2620 v3 6-core processors
- NVIDIA Tesla K80 GPU accelerator containing two Kepler GK210 GPUs
- 384 GB RAM
- 24 GB GPU RAM

The full Cooley system has:

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

DATA STORAGE

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

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

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

NETWORKING

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

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

The ALCF is actively engaged in several forward-looking activities that are helping to shape the future of supercomputing.

OUTR

SHAPING THE FUTURE OF SUPERCOMPUTING

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

ALCF researchers collaborate to help users prepare for the scale and architecture of leadership computing systems.

ALCF leadership holds regular meetings to discuss the facility's strategic initiatives.

HPCOR

ALCF staff played a key role in DOE's High-Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance in September. Chaired by ALCF Director of Science Katherine Riley, the three-day workshop brought together application developers, computing facilities, vendors, and library and tool developers to identify approaches and best practices for increasing application portability and performance on diverse architectures in the coming years.

Exascale Requirements Reviews

ALCF is collaborating with the other DOE ASCR facilities, OLCF and NERSC, to hold a series of Exascale Requirements Reviews to determine the mission-critical computational science objectives for each of the six DOE Office of Science program offices through 2025. These workshops bring together key domain scientists and computational science experts to identify the requirements for developing an exascale ecosystem that includes computation, data analysis, software, workflows, HPC services, and other features. The reviews for High Energy Physics and Basic Energy Sciences were held in 2015, with the four remaining reviews planned for 2016.

IXPUG

The ALCF's next supercomputers, Aurora and Theta, will be based on successive generations of the Intel Xeon Phi processor. As one of the founding members of the Intel Xeon Phi User's Group (IXPUG), the ALCF has been active in the group's mission to provide a forum for exchanging information to enhance the usability and efficiency of scientific and technical applications running on large-scale HPC systems that use the Xeon Phi processor. ALCF Industry Outreach Lead David Martin represents the facility as member of the IXPUG Steering Committee. In 2015, the committee organized a workshop and a birds-of-a-feather (BOF) session at ISC'15, a BOF session at SC15, and the IXPUG Annual Meeting at Lawrence Berkeley National Laboratory.

The ALCF is committed to providing training and outreach opportunities that prepare researchers to efficiently use its leadership computing systems, while also cultivating a diverse and skilled HPC workforce for the future.

GROWING THE HPC COMMUNITY

ALCF researcher William Scullin (right) provides a facility tour to a group of early-career nuclear engineers.

ENGAGING STUDENTS

Hour of Code

As part of Code.org's annual Hour of Code event in December, several ALCF staff members visited Chicago-area schools to spark interest in computer science and coding. Working with classrooms ranging from kindergarten to high school, the ALCF volunteers led a variety of activities designed to demystify code and show that anybody can learn the basics. The global outreach campaign aims to expand participation and increase diversity in computer science. ALCF participants included Liza Booker, Lisa Childers, Kevin Harms, Sunhwan Jo, David Martin, Michael Papka, Jini Ramprakash, and Khairi Reda.

Summer Coding Camp

For another computer science education effort, Argonne hosted a summer coding camp with 42 students from Chicago-area high schools. The four-day event covered an introduction to the Python programming language, emphasized problem-solving skills, and showed students what it's like to be a computer science professional. Joe Insley, Michael Papka, and Silvio Rizzi of the ALCF teamed up with Argonne's Educational Programs group and other computer scientists at the laboratory to develop and deliver the curriculum.

SC15 Student Cluster Challenge

The ALCF sponsored a team in the Student Cluster Competition at SC15, an annual event that challenges students teams to assemble a working cluster on the conference exhibit floor and demonstrate its performance using real scientific applications and benchmarks. With financial and technical support provided by Argonne and Intel, the Illinois Institute of Technology (ITT) team, which consisted of five IIT students and one Naperville Central High School student, built a five-node cluster with four Intel Xeon CPUs. ALCF researchers Ben Allen and William Scullin worked closely with the students to provide logistical, setup, and application support. ALCF Director Michael Papka facilitated the sponsorship, allocating staff and computing resources to the project.

Summer Student Program

Every year, the ALCF solicits project proposals from staff members who are interested in mentoring summer students. Through programs like DOE's Science Undergraduate Laboratory Internship (SULI) program and Argonne's Research Aide Appointments, college students are brought in to work alongside ALCF mentors on real-world research projects. In 2015, the facility welcomed its largest summer student class to date—a group of 24 students who ranged from college freshmen to PhD candidates. This year's crop of students tackled a wide variety of projects that covered everything from system administration and data analytics to computational science and performance engineering. The 10-week program culminated with a special seminar that allowed the students to present their project results.

Top: ALCF Director Michael Papka works with high school students at Argonne's summer coding camp.

Right: ALCF staff participated in a My Brother's Keeper event at Argonne, helping guide a group of eighth-graders through a day of computational thinking.
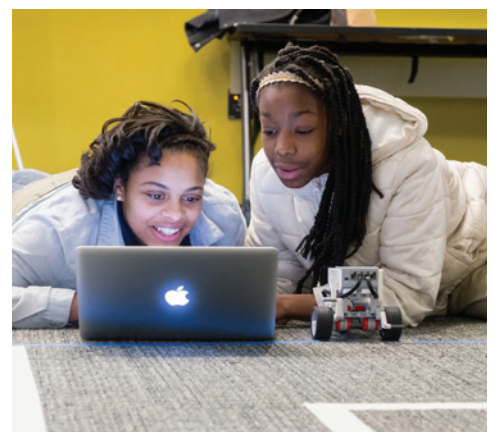
GUIDING CURRENT AND FUTURE USERS

INCREASE Workshop

This fall, Argonne partnered with the Interdisciplinary Consortium for Research and Education and Access in Science and Engineering (INCREASE) for a two-day workshop aimed at increasing the participation in and diversity of the user base at the laboratory's scientific user facilities, with a focus on engaging minority-serving institutions.

As part of the event, the ALCF held a brainstorming session to identify and better understand the barriers to gaining access to ASCR user facilities and how to overcome them. The partnership between INCREASE and Argonne has established a foundation for growing the next generation of STEM professionals and HPC users at minority-serving institutions.

ATPESC

For two weeks this summer, a group of 65 students and early career researchers attended the Argonne Training Program on Extreme-Scale Computing (ATPESC), a course designed to teach them the key skills and tools needed to efficiently use leading-edge supercomputers. Packed with technical lectures, hands-on exercises, and dinner talks, the arduous training program addresses all aspects of HPC with a curriculum that evolves each year to emphasize particular areas of interest.

This year, the organizers incorporated more hands-on sessions and placed increased focus on the importance of performance portability across diverse computing architectures.

The content was organized around seven core program tracks: hardware architectures; programming models and languages; numerical algorithms and FASTMath; community codes and software engineering; visualization and data analysis; toolkits and frameworks; and data-intensive computing and I/O. As with previous years, the ALCF recorded all of the 2015 ATPESC presentations and posted them to YouTube to extend the reach of the program.

Mira Performance Boot Camp

Now in its seventh year, the ALCF's Boot Camp event is a cornerstone of the facility's user training program. The three-day on-site workshop provides a timely opportunity for the user community to tap into the expertise of assembled ALCF staff and invited guests for help ramping up their code's scalability as they prepare to submit a proposal for an INCITE award.

The bulk of this year's event was devoted to hands-on, one-on-one tuning of applications. In addition, ALCF experts spoke on topics of interest, including Blue Gene/Q architecture, ensemble jobs, parallel I/O, and data analysis. Guest speakers from tool and debugger vendors provided information and individualized assistance to attendees.

Reservation queues created specifically for the event gave the participants quick, uninterrupted access to ALCF resources, allowing them to run 835 jobs and to use more than 18.8 million core-hours as they diagnosed code issues and tweaked performance. This year, several groups were able to complete full-machine runs on Mira and generate plots to incorporate into their INCITE proposals.

Virtual Training for Users

Employing an interactive videoconference format, the ALCF is able to connect with users from around the globe to provide virtual training on ALCF services and resources.

Offered several times a year, the Getting Started on ALCF Resources videoconference is targeted at new users and those in need of a refresher. The highly interactive sessions cover the basics that researchers need to get their projects up and running, and give users an opportunity to receive guided assistance in building their codes and submitting jobs on Mira.

New in 2015, the Ensemble Jobs for Better Throughput videoconference was developed for users whose workloads include multiple small jobs (<8K nodes) that are suitable to run concurrently. The specialized training session gave participants hands-on experience setting up an ensemble job script and helped them identify which job submission type is best for their projects.

The ALCF also used the virtual format for the Theta Early Science Program, holding videoconferences with project teams for the kickoff workshop and the program's first training session.

From introducing students to exciting career possibilities in HPC to working with users to inform them of new approaches for leadership-class systems, education is a critical part of the ALCF's mission.

ALCF held or participated in a number of training and outreach events in 2015, including the Mira Performance Boot Camp (top), ATPESC (middle left), Getting Started videoconferences (middle right), and the INCREASE workshop (bottom).

APPENDICES

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 in descending order of their publication dates. An asterisk after a name indicates an Argonne author. ALCF publications are listed online at http://www.alcf.anl.gov/publications.

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ALCF PROJECTS

2015 INCITE PROJECTS

Biological Sciences

**Multiscale Simulations
of Human Pathologies**
George Karniadakis
Brown University
70 Million Core-Hours
(ALCF: 45M; OLCF: 25M)

**Studies of Large Conformational
Changes in Biomolecular Machines**
Benoît Roux
The University of Chicago
120 Million Core-Hours

Chemistry

Catalyst Support Interactions
Frank Abild-Pedersen
Stanford University
50 Million Core-Hours

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

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

Computer Science

**Dynamic and Adaptive Parallel
Programming for Exascale Research**
Robert Harrison
Brookhaven National Laboratory
15 Million Core-Hours

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

**Scalable System Software
for Parallel Programming**
Robert Latham
Argonne National Laboratory
25 Million Core-Hours

Earth Science

**Accelerated Climate Modeling
for Energy**
Mark Taylor
Sandia National Laboratories
190 Million Core-Hours
(ALCF: 140M; OLCF: 50M)

**CESM Century-Scale
Climate Experiments with
a High-Resolution Atmosphere**
Warren Washington
National Center for
Atmospheric Research
200 Million Core-Hours
(ALCF: 200M; OLCF: 0)

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

**High Frequency Ground
Motion Simulation for
Seismic Hazard Analysis**
Thomas Jordan
University of Southern California
167 Million Core-Hours
(ALCF: 48M; OLCF: 119M)

Engineering

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

**Direct Numerical Simulations
and Robust Predictions
of Cloud Cavitation Collapse**
Petros Koumoutsakos
Swiss Federal Institute of Technology
88 Million Core-Hours

**DNS/LES of Complex
Turbulent Flows**
Krishnan Mahesh
University of Minnesota
100 Million Core-Hours

**Large-Eddy Simulations
of Combustor Liner Flows**
Anne Dord
GE Global Research
89 Million Core-Hours

**Large-Eddy Simulation
of the Bachalo-Johnson Flow,
with Shock-Induced Separation**
Philippe Spalart
Boeing
135 Million Core-Hours

**Parameter Studies
of Boussinesq Flows**
Susan Kurien
Los Alamos National Laboratory
44 Million Core-Hours

Materials Science

**Computational Spectroscopy
of Heterogeneous Interfaces**
Giulia Galli
The University of Chicago
180 Million Core-Hours

**Non-Covalent Bonding
in Complex Molecular Systems
with Quantum Monte Carlo**
Dario Alfè
University College London
148 Million Core-Hours
(ALCF: 68M; OLCF: 80M)

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

**Predictive Materials Modeling
for Li-Air Battery Systems**
Larry Curtiss
Argonne National Laboratory
50 Million Core-Hours

**QMC Simulations DataBase for
Predictive Theory and Modeling**
David Ceperley
University of Illinois
at Urbana–Champaign
185 Million Core-Hours
(ALCF: 100; OLCF: 85)

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

**Simulation of Correlated Electrons
for Superconducting Materials**
Lucas Wagner
University of Illinois
at Urbana–Champaign
106 Million Core-Hours

**SiO2 Fracture: Chemomechanics
with a Machine Learning Hybrid
QM/MM Scheme**
James Kermode
King's College London
125 Million Core-Hours

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

Physics

Accelerator Modeling for Discovery
James Amundson
Fermilab
60 Million Core-Hours

Cosmic Reionization on Computers
Nickolay Gnedin
Fermilab
74 Million Core-Hours

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

**High-Fidelity Simulation
of Tokamak Edge Plasma Transport**
Choong-Seock Chang
Princeton Plasma Physics Laboratory
270 Million Core-Hours
(ALCF: 100M; OLCF: 170M)

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

**Nuclear Structure
and Nuclear Reactions**
James Vary
Iowa State University
204 Million Core-Hours
(ALCF: 100M; OLCF: 104M)

**Particle Acceleration in Shocks:
From Astrophysics to Laboratory
In Silico**
Frederico Fiuza
SLAC National Accelerator Laboratory
110 Million Core-Hours

**Petascale Simulation
of Magnetorotational
Core-Collapse Supernovae**
Sean Couch
Michigan State University
50 Million Core-Hours

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

**Quark Flavors and Conserved
Charges at Finite Density
in the QCD Phase Diagram**
Rene Bellwied
University of Houston
150 Million Core-Hours

2014 ALCC PROJECTS

Biological Sciences

**Applying Breakthroughs in Protein
Structure Calculation to the Creation
of Designer Enzymes**
David Baker
University of Washington
200 Million Core-Hours

Chemistry

**Influence of Morphology
on Proton Transport
in Proton Exchange Membrane**
Gregory Voth
The University of Chicago/
Argonne National Laboratory
57.6 Million Core-Hours

**Large-Scale Turbulent
Clean Coal Combustion**
Martin Berzins
University of Utah
40 Million Core-Hours
(ALCF: 10M; OLCF: 30M)

Computer Science

**Hobbes: Operating System and
Runtime Research for Extreme Scale**
Ron Brightwell
Sandia National Laboratories
40 Million Core-Hours
(ALCF: 5M; NERSC: 5M; OLCF: 30M)

Earth Science

Delivering the Department of Energy's Next-Generation High-Resolution Earth System Model
Peter Thornton
Oak Ridge National Laboratory
137 Million Core-Hours
(ALCF: 107M; OLCF: 30M)

Engineering

Amplitude Modulation of Wind Turbine Noise
Sanjiva Lele
Stanford University
36.5 Million Core-Hours

Petascale Simulations in Support of CESAR
Elia Merzari
Argonne National Laboratory
80 Million Core-Hours

Predictive Large-Eddy Simulation of Jet Fuel Atomization, High-Lift Airframes, and Reacting Supersonic Turbulent Flows on Unstructured Grids
Parviz Moin
Stanford University
120 Million Core-Hours

Understanding Secondary Motions and Their Impact in Modeling Turbulent Flows
Hassan Nagib
Illinois Institute of Technology
11 Million Core-Hours

Materials Science

Interfaces in Organic and Hybrid Photovoltaics
Noa Marom
Tulane University
105 Million Core-Hours
(ALCF: 75M; NERSC: 30M)

Large-Scale Quantum Simulations of Electrode-Electrolyte Interfaces
Giulia Galli
The University of Chicago
35 Million Core-Hours

Nanostructure-Enhanced Chemical Reactivity and Detonation in Energetic Materials
Aidan Thompson
Sandia National Laboratories
80 Million Core-Hours

Prediction and Design of Energy Materials by Petascale Evolutionary Algorithm Simulations
Giancarlo Trimarchi
Northwestern University
30 Million Core-Hours

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

Physics

Composite Higgs Theory Beyond the Standard Model and the 14 TeV Upgrade of the Large Hadron Collider
Julius Kuti
University of California, San Diego
88.7 Million Core-Hours

Cosmic Frontier Computational End-Station
Salman Habib
Argonne National Laboratory
176 Million Core-Hours
(ALCF: 100M; NERSC: 76M)

Ion Solvation, Catalytic Interfaces, and Extreme Aqueous Environments: An *Ab Initio* Study of Liquid Water
Robert A. DiStasio Jr.
Cornell University
350 Million Core-Hours

Simulation of Large Hadron Collider Events Using Leadership Computing
Thomas LeCompte
Argonne National Laboratory
52 Million Core-Hours
(ALCF: 50M; NERSC: 2M)

Turbulent Multiphase Flows for Nuclear Reactor Safety
Igor A. Bolotnov
North Carolina State University
76.8 Million Core-Hours

Understanding Helium Plasma Mediated Tungsten Surface Response to Better Predict Fusion Plasma Facing Component Performance in ITER
Brian Wirth
University of Tennessee
96 Million Core-Hours
(ALCF: 66M; OLCF: 30M)

Validation Studies of Gyrokinetic Simulations to Understand the Coupling of Ion and Electron Scale Turbulence in Tokamak Plasmas
Christopher Holland
University of California, San Diego
140 Million Core-Hours
(ALCF: 90M; NERSC: 50M)

2015 ALCC PROJECTS

Chemistry

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

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

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

Computer Science

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

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

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

Earth Science

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

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

Engineering

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

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

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

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

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

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

Materials Science

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

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

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

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

Physics

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

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

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

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

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

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

2015 DIRECTOR'S DISCRETIONARY PROJECTS

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

Biological Sciences

Binding Affinity Calculations of Estrogen Receptor Against FDA-Approved Drugs
Sichun Yang
Case Western Reserve University
8 Million Core-Hours

Computing Three-Dimensional Structures of Large RNA from Small Angle X-Ray Scattering Data and Secondary Structure
Yun-Xing Wang
National Cancer Institute
15 Million Core-Hours

Correlating Experimentally Measured Molecular Dynamics with Computational Trajectories: Understanding Dynamic Allostery in Ubiqu
R. Andrew Byrd
National Cancer Institute
5 Million Core-Hours

Developing Novel Umbrella Sampling/Solute Tempering Algorithms in NAMD
Sunhwan Jo
Argonne National Laboratory
4.1 Million Core-Hours

Highly Parallel Macromolecular Conformational Searches and Energy Evaluations with the CHARMM Program
Robert J. Petrella
Harvard University
10 Million Core-Hours

Long-Time MD Simulation of Protein Structural Function
Ruth Nussinov
National Cancer Institute
2 Million Core-Hours

Virus Calculations with FMO
Yuri Alexeev
Argonne National Laboratory
15 Million Core-Hours

Chemistry

Large-Scale Combustion Preparatory Access
Gabriel Staffelbach
CERFACS
12 Million Core-Hours

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

Quantum Monte Carlo Applied to Lithium Hyperoxides in Li-Air Batteries
John J. Low
Argonne National Laboratory
10 Million Core-Hours

Shift-and-Invert Parallel Spectral Transformation Eigensolver
Murat Keceli
Argonne National Laboratory
500,000 Core-Hours

Solving Petascale Public Health & Safety Problems Using Uintah
Martin Berzins
University of Utah
1 Million Core-Hours

Computer Science

ExaHDF5: Advancing HDF5 HPC I/O to Enable Scientific Discovery
Venkatram Vishwanath
Argonne National Laboratory
5 Million-Core Hours

Performance Studies of Three-Dimensional Fast Fourier Transforms Using Overlap of Communication with Computation
Dmitry Pekurovsky
University of California, San Diego
2.5 Million Core-Hours

SciDAC Scalable Data Management Analysis and Visualization
Michael E. Papka
Argonne National Laboratory
3.25 Million Core-Hours

Earth Science

Scalability Study for NUMA (Non-Hydrostatic Unified Model of the Atmosphere)
Andreas Mueller
Naval Postgraduate School
5 Million Core-Hours

Energy Technologies

GTRI- and NEAMS-Related Production Tests and Runs
Micheal A. Smith
Argonne National Laboratory
10 Million Core-Hours

Engineering

Aircraft Fuel Burn Reduction Using Minute Roughness Elements
Ali Uzun
Florida State University
1 Million Core-Hours

DNS of Compressible Turbulent Boundary Layers
Jonathan Poggie
Air Force Research Laboratory
5 Million Core-Hours

DNS of Multi-Mode Rayleigh-Taylor Instability
Maxwell Hutchinson
The University of Chicago
5 Million Core-Hours

Extreme-Scale Unstructured Mesh CFD Workflow
Cameron Smith
Rensselaer Polytechnic Institute
5 Million Core-Hours

Large-Eddy Simulation of Crackling Supersonic Jets
Joseph Nichols
University of Minnesota
10 Million Core-Hours

Numerical Simulation of Acoustic Radiation from High-Speed Turbulent Boundary Layers
Lian Duan
Missouri University
of Science and Technology
2 Million Core-Hours

Performance Improvement of CFD Code CONVERGE on BG/Q Systems
Marta García and Sibendu Som
Argonne National Laboratory
6 Million Core-Hours

Primary Atomization DNS of ECN's Spray A
Marcus Herrmann
Arizona State University
5 Million Core-Hours

Turbulent Rayleigh-Benard Convection at High Rayleigh and Low Prandtl Numbers
Janet Scheel
Occidental College
1 Million Core-Hours

Materials Science

Collective I/O and Bond Analysis Code Development on SiC Nanoparticle Oxidation
Ying Li
Argonne National Laboratory
5 Million Core-Hours

Electronic Response to Particle Radiation in Semiconductor Systems
Andre Schleife
University of Illinois
at Urbana-Champaign
16 Million Core-Hours

High-Performance Li-Air Battery
Ying Li
Argonne National Laboratory
5 Million Core-Hours

Integrating Simulation and Observation: Discovery Engines for Big Data
Justin Wozniak
Argonne National Laboratory
6.9 Million Core-Hours

Many-Body Stochastic Analysis of Semiconductor Bulk and Defect Properties
Elif Ertekin
University of Illinois
at Urbana-Champaign
2 Million Core-Hours

Mathematics

Parallel Multiscale Simulations of Advanced Steel Materials
Axel Klawonn
University of Cologne; Oliver Rheinbach, Technische Universität Bergakademie Freiberg
3 Million Core-Hours

Scalable Domain Decomposition Methods for Computational Cardiology and Isogeometric Analysis
Luca F. Pavarino
University of Milan
1.3 Million Core-Hours

Physics

Calculation of Nuclear Matrix Element of Neutrinoless Double-Beta Decay
Jun Terasaki
University of Tsukuba
3.8 Million Core-Hours

DNS Simulations of Turbulent Rayleigh-Taylor Unstable Flames Using Nek5000
Elizabeth P. Hicks
Epsilon Delta Labs
2.5 Million Core-Hours

Effective Interactions in Coulombic Systems with Highly Disparate Particle Sizes
Monica Olvera de la Cruz
Northwestern University
3.1 Million Core-Hours

Extreme-Scale Turbulence Simulations
William M. Tang
Princeton Plasma Physics Laboratory
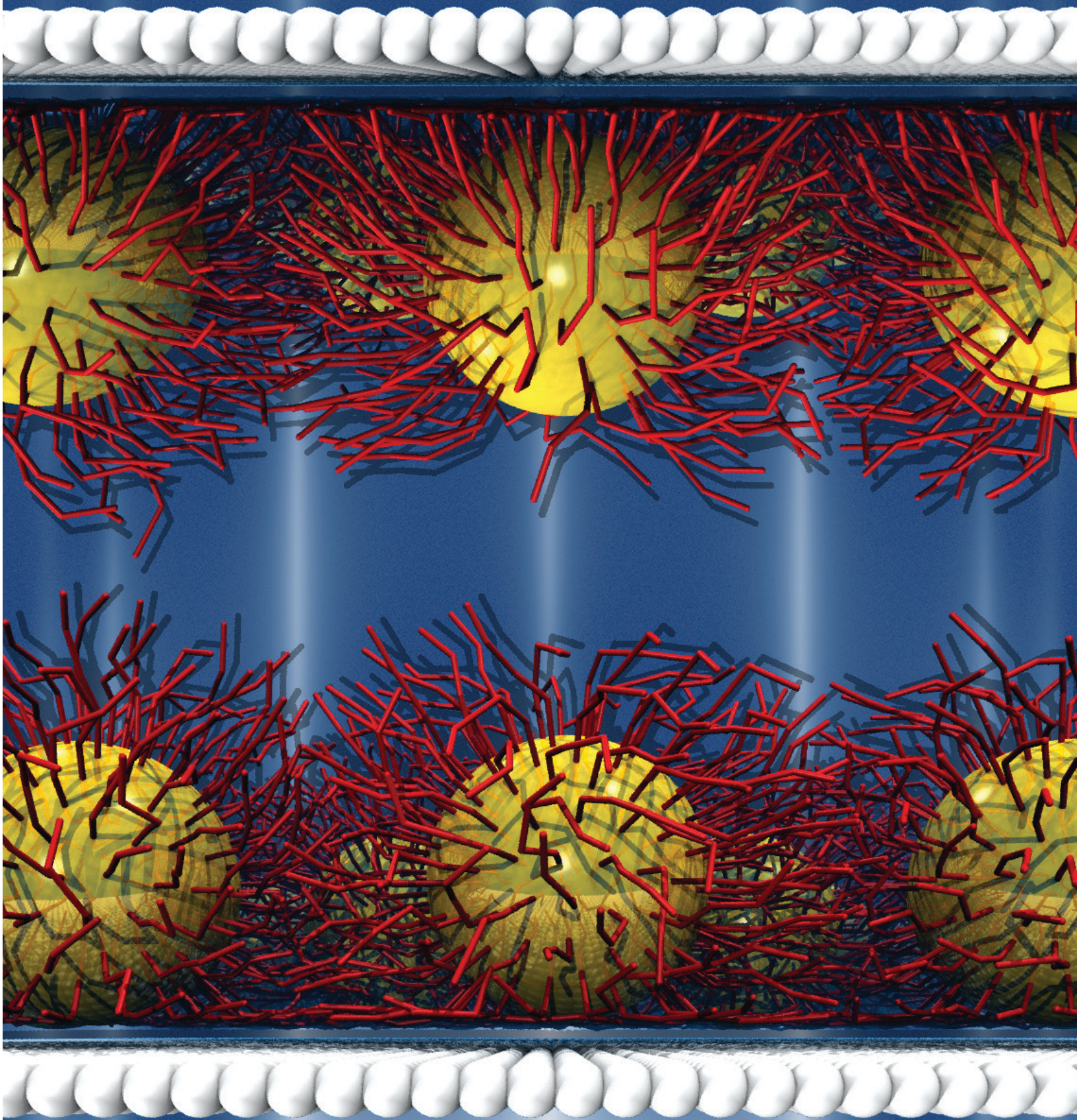60 Million Core-Hours

Mira Simulations of High-Intensity Laser Experiments to Study Turbulent Amplification of Magnetic Fields
Don Q. Lamb
The University of Chicago
10 Million Core-Hours

Moving Mesh Simulations of Gravito-Turbulence in Global Proto-Planetary Disks
Andrew MacFadyen
New York University
250,000 Core-Hours

An illustration of self-assembled gold (yellow spheres) nanoparticle monolayers on supporting interfaces (white spheres) showing preferential asymmetry in ligand (red sticks) coverage.

Image credit: Joseph A. Insley and Subramanian Sankaranarayanan, Argonne National Laboratory

About Argonne Leadership Computing Facility

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

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