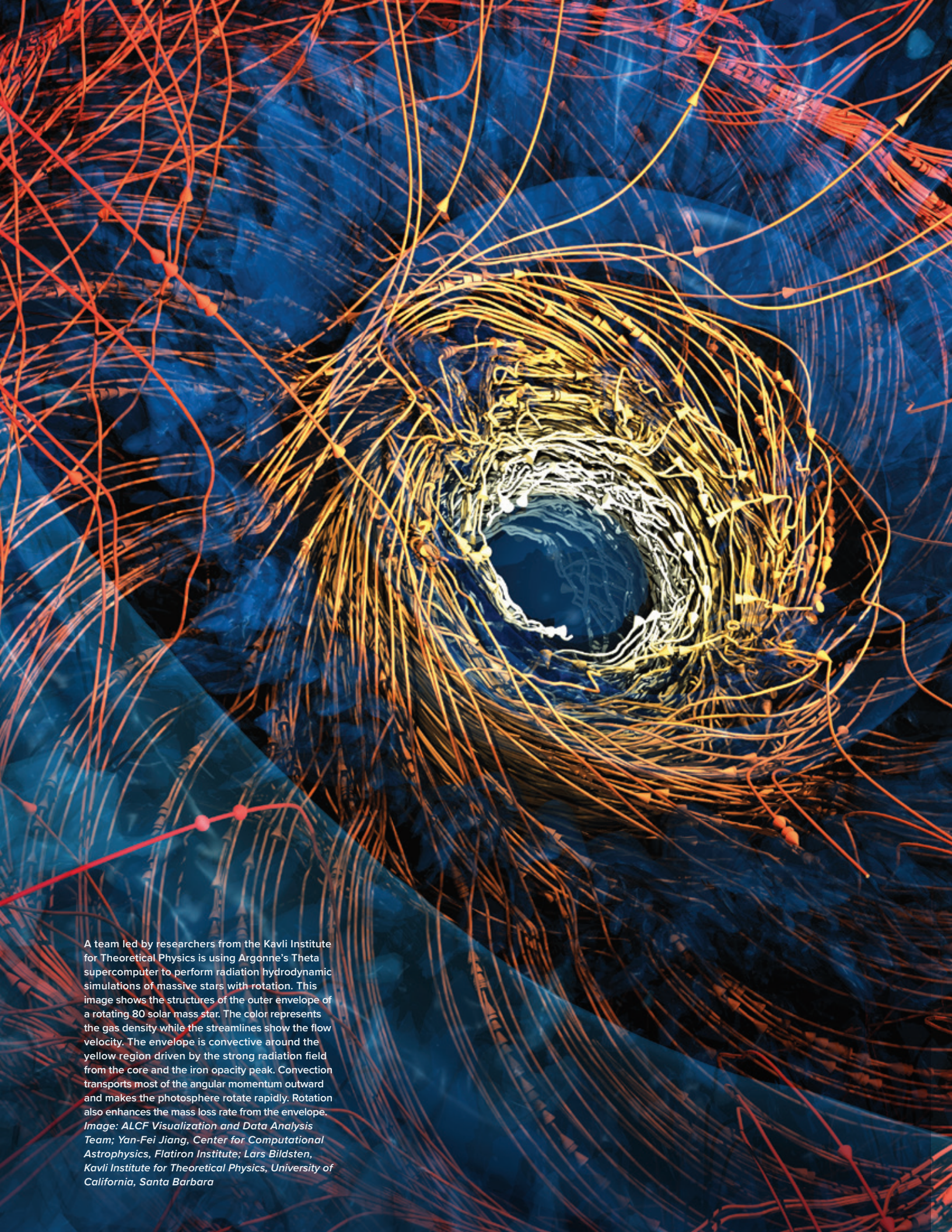
Argonne NATIONAL LABORATORY

Argonne Leadership Computing Facility

2021 Annual Report



A team led by researchers from the Kavli Institute for Theoretical Physics is using Argonne's Theta supercomputer to perform radiation hydrodynamic simulations of massive stars with rotation. This image shows the structures of the outer envelope of a rotating 80 solar mass star. The color represents the gas density while the streamlines show the flow velocity. The envelope is convective around the yellow region driven by the strong radiation field from the core and the iron opacity peak. Convection transports most of the angular momentum outward and makes the photosphere rotate rapidly. Rotation also enhances the mass loss rate from the envelope. *Image: ALCF Visualization and Data Analysis Team; Yan-Fei Jiang, Center for Computational Astrophysics, Flatiron Institute; Lars Bildsten, Kavli Institute for Theoretical Physics, University of California, Santa Barbara*

CONTENTS

2021 Annual Report

02 Year in Review

04 ALCF Director's Message
06 ALCF Leadership
10 ALCF at a Glance

12 Charting Future Directions in Scientific Computing

14 Making Data a First-Class Citizen
18 Integrating the ALCF with Experimental Facilities
20 Polaris to Help Pave the Way to Exascale
22 The Road to Aurora

32 Growing the HPC Community

34 Creating a Diverse and Inclusive Workplace
38 Partnering with Industry
40 Shaping the Future of Supercomputing
44 Engaging Current and Future HPC Users

50 Expertise and Resources

54 ALCF Systems
56 ALCF Team

62 Science

64 Accessing ALCF Resources for Science

66 Finding Druggable Sites in SARS-CoV-2 Proteins Using Molecular Dynamics and Machine Learning
Albert Lau

67 Observing the SARS-CoV-2 Replication-Transcription Machinery in Action
Arvind Ramanathan

68 DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications
Huihuo Zheng
Venkatram Vishwanath

69 Automatic Building Energy Modeling
Joshua New

70 ExaSMR: Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors
Steve Hamilton

71 Dynamic Compressed Sensing for Real-Time Tomographic Reconstruction
Robert Hovden

72 Towards Automated Discovery and Optimization of Spin Defects for Quantum Technologies
Giulia Galli

73 Towards Predictive Simulations of Functional and Quantum Materials
Paul Kent

74 Ultrafast Control of Functional Materials
Priya Vashishta

75 Amplification of Cosmic Magnetic Fields Captured in Laser Experiments
Petros Tzeferacos

76 High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics
Choong-Seock Chang

77 Mira's Last Journey
Katrin Heitmann

78 ALCF Projects
82 ALCF Publications

YEAR IN REVIEW

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

Components of the ALCF's Aurora exascale system were delivered in 2021.

ALCF Director's Message

MICHAEL E. PAPKA
ALCF Director

Computational investments are but one aspect of what makes ALCF a leadership facility. We also serve as a unique and evolving provider of new capabilities, services, training, and support, and our ability to match resources to the needs of our user community requires immense planning and foresight. We believe our future as a facility will be determined by data—not its growth, per se, rather data generated by many and varied sources—from simulation, analysis, experiments, and beyond. Our future is about the organization, sharing, and evaluation of data.

Moving forward, we are looking at new ways to interrogate and enhance scientific datasets. This presents a different set of challenges—and, for advanced computing facilities like ours, exciting opportunities. HPC users are always making new demands of their data—from performing analysis in situ, to supporting real-time collaborations—and scientific use cases are a great way to understand new ways of managing scientific data to discover things, faster.

To support this future, we deployed our two largest storage systems yet: Grand, named for the Grand Canyon, and Eagle, for the Eagle River. These two 100-petabyte systems will support our user community for years to come, bringing new services and powering data-driven research. We recently implemented production data sharing via Globus on Eagle and have initiated the ALCF Community Data Co-Op (ACDC). The ACDC portal will be a platform for sourcing and exchanging datasets while also preserving them for future analysis, extending their utility and reach to other research groups and other areas of science.

In 2021, ALCF began deploying Polaris, our newest 40-petaflops system, to help us prepare for our future Intel-HPE exascale system, Aurora. We also outfitted Polaris with 28 additional nodes to support the integration of experiments and HPC resources. With this new capacity, scientists can begin to access and analyze data from their live experiments, in real time and as needed to correct any initial errors. In the months to come, Polaris will take on use cases originating at the Advanced Photon Source and other facilities to better understand the challenges and demands of extensive experiments that require immediate access to a machine, skipping over days or weeks of regularly scheduled queues.

Of course, Polaris itself is a platform for debugging and optimizing scientific codes for Aurora, a machine that will simultaneously manage simulation data, machine learning and deep learning tasks, and data science workloads, in new and exciting ways.

Among the successes afforded by our steady state resources, Theta delivered over 20 million node-hours alone to 16 INCITE projects and more than 7 million node-hours to 49 ALCC projects, advancing studies ranging from designing future fusion reactors, to finding druggable sites in SARS-CoV-2 proteins, to expanding the scale of urban building energy modeling.

Argonne's Joint Laboratory for System Evaluation (JLSE) continued to operate advanced testbeds used to both prepare for Aurora and support more than 80 projects ranging from application portability to software development to tools and compiler development. ALCF's AI Testbed, launched in 2020 to allow Argonne researchers to experiment in the accelerator space, is now preparing to open to the entire research community.

Our future as a facility is being shaped by all our activities, but especially by our interest in the future of data. And the future of data is about more than just machine resources; it's also about services that distribute data and increase its usefulness to the larger scientific community.

And, as always, our future is tied to the incredible workforce we will continue to attract. And we have continued to expand this pipeline through our diversity, equity, and inclusion (DEI) initiatives, our partnerships with local universities, the training programs we conduct, the research appointments we support, and the fellowships we sponsor.

This Annual Report showcases the big milestones we've reached as a facility on the path to a brighter future, measured by how, and how well, we can enable our users to do high-impact science.

ALCF Leadership

SUSAN COGHLAN
ALCF-X Project Director

2021 was a year like no other—OK, it was a bit like 2020. But as the world was encouraging us to stay apart, I am happy to report that our team came together safely for one of ALCF's most productive years ever. Not only did we continue to operate a world-class computing facility, we also completed several major projects and took a big step toward delivering our exascale computer, Aurora. We completed the expansion of the Theory and Computing Sciences (TCS) data center to add 15,000 square feet of floor space for Aurora and its supporting hardware. We also completed the mechanical and electrical space construction in collaboration with TCS Building Trust and Turner Construction. We have even started to receive Aurora components that will be installed in 2022.

On the technical side, we deployed early spins of the discrete Intel GPUs (Intel XeHP SDV GPUs) in a system called Arcticus. The Arcticus GPUs are the generation prior to the Intel GPUs (code named Ponte Vecchio or PVC for short) that will power Aurora. Arcticus proved to be a great platform for the Early Science Program and Exascale Computing Project teams working to develop, debug, and begin optimizing their codes for Aurora. In addition, the ALCF-3 team gained access to very early spins of PVC at Intel and was able to make progress in testing applications and running benchmarks on the GPUs. Early spins of PVC will be deployed at Argonne in the Florentia system in the first quarter of 2022.

For a year that tried to keep us apart, the ALCF-3 project team came together to do some fantastic things—laying the groundwork for a busy but exciting 2022 as we get ready to turn on Argonne's first exascale resource.

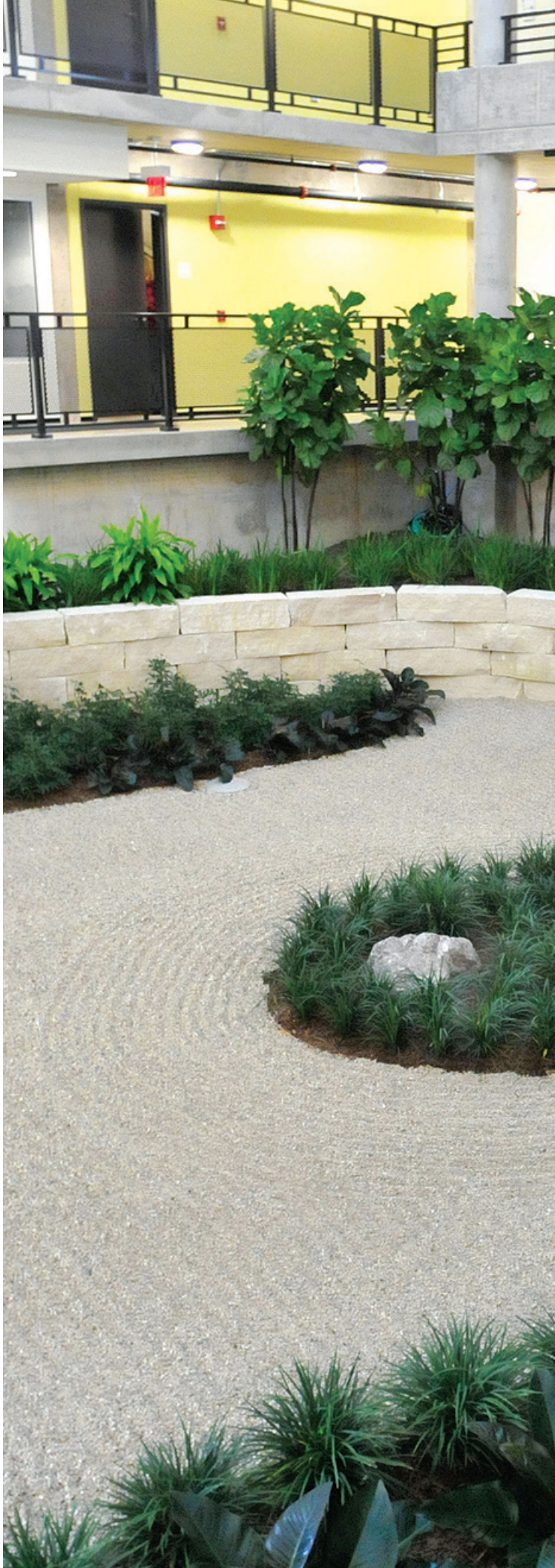
MARK FAHEY
ALCF Director of Operations

Polaris, a 560-node HPE Apollo 6500 Gen10+ based-system, was delivered in July. The new platform, equipped with AMD EPYC CPUs and NVIDIA A100 GPUs, will allow researchers to gain early experience with Aurora-like technologies while simultaneously providing a resource for users to explore AI and machine learning for science.

On January 1, we deployed two 100 PB file systems, named Grand and Eagle, providing 650 GB/s bandwidth each. Eagle was configured to allow principle investigators to set up community data sharing with Globus. With this ability, PIs can now share their data with communities outside of ALCF. Collaborators can both read and store data in the shared spaces. We also worked closely with Globus to add anonymous https read-only controls—a feature many projects are interested in.

Although Mira was decommissioned in 2020, the Mira project filesystems remained in production until late this year. These filesystems were extremely stable and productive, giving the ALCF user community trusted project space. The planning and execution of the decommissioning of 27 racks with 12,320 disks will complete early next fiscal year.

We also continue to contribute to the OpenPBS community on scheduler developments. The new resources deployed at ALCF starting with Polaris will use PBS, which will feel quite similar to Cobalt while providing new features that will take full advantage of the upcoming heterogeneous architectures. Additions to OpenPBS include new scheduler events that allow us to drive our reporting framework. The recent focus has been on implementing our scheduling policies in PBS in preparation for our first production deployments. We have been providing feedback on the REST/GraphQL interfaces, and our next planned feature addition will be around adding flexibility to reservations.



KALYAN KUMARAN
ALCF Director of Technology

In 2021, we continued preparing for Aurora through collaborations with Intel on the non-recurring engineering (NRE) contract and by working closely with several teams participating in DOE's Exascale Computing Project (ECP) and the Aurora Early Science Program (ESP). Our team was also involved in the early testing and acceptance preparation for Polaris, gaining valuable experience ahead of Aurora's arrival. The collaborative efforts led to a number of highlights: standing up the Aurora testbeds, Arcticus and Presque, for ESP and ECP users at JLSE; making significant progress in oneAPI development especially in compilers, math libraries and AI frameworks; and advancing application porting efforts for Aurora. To push portable programming models across various ecosystems, the team worked on supporting SYCL and HIP on all DOE supercomputers.

We also made a concentrated effort to provide more training opportunities to prepare users for Aurora and Polaris. Topics for the ALCF's monthly webinars specifically targeted the programming models, performance tools, I/O, and AI software that will be available on these systems. Our team also led workshops and sessions on SYCL/DPC++ and DAOS at computing events like SC21 and the ECP Annual Meeting.

In the AI space, our staff contributed to the MLPerf HPC and Science benchmarks. The team also initiated the ALCF AI for Science Training Series to teach a new generation of researchers how to use supercomputers for AI research. We continued to grow the ALCF AI Testbed, adding new AI accelerators and conducting several workshops on how to effectively use the systems for science.

Overall, I'm proud to say the team has adapted well to work in a virtual environment and continues to support our users in their pursuit of scientific discoveries.

JINI RAMPRAKASH
ALCF Deputy Director

KATHERINE RILEY
ALCF Director of Science

Remote work was the norm for a second consecutive year in 2021. While some on-site work was required, a majority of the ALCF team continued to connect and collaborate via Zoom, Slack, and other online communications tools. Among the virtual activities, we successfully hosted our Operational Assessment Review over Zoom in March. We also participated in a new collaborative effort with the DOE Office of Science aimed at building an integrated research infrastructure across DOE user facilities to accelerate discoveries. As a first step, we worked with our sister facilities to produce a white paper detailing the operational implications of integrating computing, experimental, and observational facilities.

We continue to make strides in our efforts to make diversity, equity, and inclusion an integral part of our work environment and culture. At the SIAM CSE21 conference, I served on the organizing committee for the Sustainable Horizon Institute's Broader Engagement program, which helps bring students from underrepresented backgrounds into the research world through mentoring and professional development activities. Our staff also mentored several students participating in the DuPage County Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO). The event is part of a larger national competition designed to provide African American students with pathways into potential STEM careers. I'm very proud to report that my student went on to present a research poster at the Women in Data Science and Statistics Conference and another ALCF-mentored student received an award at the national competition.

In collaboration with Intel, we helped launch the oneAPI academic pilot program to build new relationships with universities to increase the pipeline of users for Aurora. Intel also named the winners of its Great Cross-Architecture Challenge, with one of the participants winning an opportunity to work with ALCF on a oneAPI-related project.

I'm consistently impressed by the amazing work being carried out by the ALCF user community. In 2021, we saw several groundbreaking studies in areas ranging from COVID-19 drug discovery to fusion energy research to modeling the energy usage of the nation's building stock. We also continued to see a shift in how researchers are approaching computational science, with more and more projects integrating AI and learning methods into data-intensive research campaigns. With the arrival of Polaris, and Aurora coming next, we're excited to provide our user community with new supercomputing resources that are equipped with advanced capabilities to support the growing number of workflows involving simulation, data, and learning methods. To that end, the ALCF team has been doing a lot of great work to prepare researchers for our upcoming systems. From hosting training events to developing a computing environment that supports multiple portable programming models, the team is helping to ensure our systems, and the scientists who use them, will be ready for science in the exascale era.

In my first year as project manager for the INCITE program, we launched an early career track to encourage a new generation of researchers to use leadership computing resources for science. For the 2022 allocation year, we awarded a total of 51 INCITE projects at ALCF and OLCF, with nine projects coming from the early career track. Next year's allocations will also mark the first INCITE projects to gain access to Polaris, with nine research teams receiving computing time on the system.

In 2021, we also completed the search for the next recipient of the ALCF's Margaret Butler Fellowship in Computational Science. We had several outstanding applicants and look forward to bringing the new fellow on board in 2022.

ALCF at a Glance

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

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

As a key player in the nation's efforts to provide the most advanced computing resources for science, the ALCF is helping to enhance research capabilities through a convergence of simulation, data science, and artificial intelligence methods.

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

Node-hours of compute time

34M

Active projects*

375

Facility users*

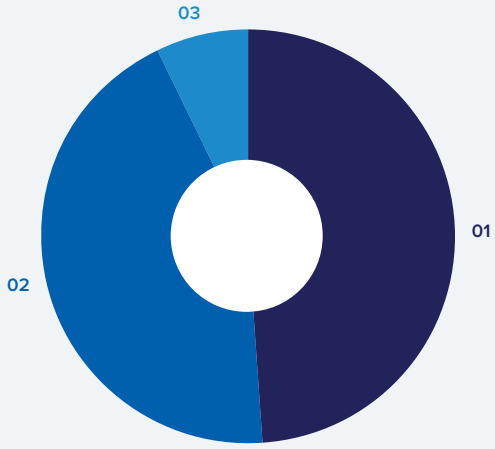
1,168

**Fiscal year 2021*

Publications

249

2021 ALCF Users by Affilliation



01 Academia

571

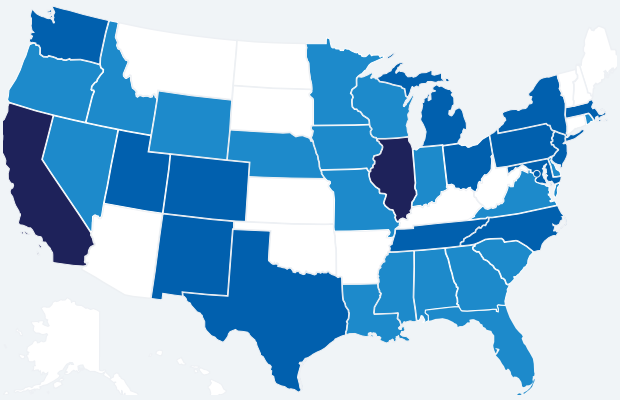
02 Government

515

03 Industry

82

2021 U.S. ALCF Users by State



100+ Users

California
Illinois

11–100 Users

Colorado
Washington D.C.
Maryland
Massachusetts
Michigan
North Carolina
New Jersey
New Mexico
New York
Ohio
Pennsylvania
Tennessee
Texas
Utah
Washington

01–10 Users

Alabama
Delaware
Florida
Georgia
Idaho
Indiana
Iowa
Louisiana
Minnesota
Mississippi
Missouri
Nebraska
Nevada
Oregon
Rhode Island
South Carolina
Virginia
Wisconsin
Wyoming

CHARTING FUTURE DIRECTIONS IN SCIENTIFIC COMPUTING

The ALCF continues to expand its capabilities to support pioneering research at the intersection of simulation, data, and learning.

Susan Coghlan, ALCF-X Project Director, accepts the delivery of the first Aurora hardware components to arrive at Argonne National Laboratory.

Making data a first-class citizen

The ALCF is creating a data-centric computing environment that enhances researchers' ability to manage, analyze, and share increasingly large scientific datasets.

Data is the lifeblood of science, providing a foundation for developing and testing new ideas that advance our understanding of the universe across all disciplines.

The pace of discovery, however, is increasingly constrained by the growing deluge of scientific data. Powerful research tools, such as supercomputers, light sources, telescopes, particle accelerators, and sensors, generate massive amounts of data each day. And as these instruments continue to evolve and improve over time, the output of data will only continue to increase. The scientific community's ability to store, process, analyze, share, and reuse such datasets is critical to gaining insights that will spark new discoveries and innovation.

To align with these emerging data management needs, the ALCF continues to expand its scope beyond that of a traditional supercomputing facility. From deploying a new portal for data sharing to building a testbed of AI accelerators for data-intensive science, the ALCF is extending the reach of its leadership computing resources by making data a first-class citizen.

ALCF Community Data Co-Op Provides Portal for Data Sharing and Discovery

While the ALCF has always had large-scale storage systems for its user community, sharing and processing the data with external collaborators has been challenging. In 2015, the ALCF introduced Petrel, a pilot data service designed to break down the barriers of large-scale data sharing with the larger research community. Developed in partnership with Globus, Petrel demonstrated the viability of a service that enabled rapid, reliable, and secure sharing of vast amounts of data from both simulations and experiments.

In 2021, the ALCF Community Data Co-Op (ACDC) replaced Petrel, providing an enhanced portal for data access and discovery. With the new Eagle global filesystem and the Globus service as its backbone, ACDC allows researchers to build out different modalities for data use, such as indexing of data for discovery, data portals for interactive search and access, and web accessible analysis services.

ACDC users can grant access to external collaborators through various application programming interfaces (APIs). The interactivity permitted by the APIs presents users with many possibilities for data control and distribution, and direct connections to high-speed external networks permit data access at many gigabytes per second.

ACDC's fully supported production environment is the next step in the ALCF's expansion of edge services that blur the boundaries between experimental laboratories and computing facilities. By enabling data sharing and access on a grand scale, the service provides a resource for researchers to discover and reuse existing datasets for additional scientific inquiries, opening the door to new breakthroughs.

ALCF AI Testbed Aims to Accelerate Data-Driven Science

AI and data go hand in hand. AI requires large volumes of data to learn. At the same time, AI techniques, such as machine learning, deep learning, and natural language processing, can help researchers accelerate data analysis to quickly pinpoint trends and patterns that lead to new insights.

Continuing Argonne's efforts to advance the use of AI for science, the ALCF is building a powerful testbed that comprises some of the world's most advanced AI accelerators. Designed to explore the possibilities of next-generation computing architectures, the ALCF AI Testbed will enable the facility and its user community to help define the role of AI accelerators in scientific research.

Offering architectural features that support AI and data-centric workloads, the testbed provides another resource that can help researchers analyze the growing amount of data produced by large-scale simulations and experiments. Moreover, the testbed components stand to significantly broaden analytic and processing abilities in the project workflows deployed at the ALCF beyond those supported by traditional CPU- and GPU-based machines.

The ALCF AI Testbed will also facilitate further collaborations with Argonne's Data Science and Learning, Mathematics and Computer Science, and Computational Science divisions, as well as the larger laboratory community.

The ALCF's new storage systems, Eagle and Grand, provide facility users with increased storage capacity and enhanced data sharing capabilities.

The ALCF AI Testbed's Cerebras CS-2 system.

The ALCF AI Testbed's SambaNova DataScale system.

Such collaborations simultaneously deepen scientific discovery while validating and establishing the capabilities of new hardware and software using real data.

While the ALCF plans to make the testbed systems available to the broader scientific community in 2022, researchers at Argonne have already began leveraging the AI accelerators for data-intensive studies in areas such as COVID-19 drug discovery, multiphysics simulations of massive stars, and cancer research.

Building a Hub for Data-Centric Computing

The launch of ACDC and the ALCF AI Testbed are critical pieces of the ALCF's vision to build a robust and interconnected computing environment for data-driven science, but the facility's evolution has been several years in the making.

In the research space, the ALCF has made a commitment to supporting projects involving data science and AI methods, such as machine learning and deep learning. In 2016, the facility launched its ALCF Data Science Program (ADSP), which aims to build a community of researchers who can use AI and data analysis methods at a scale that requires DOE's leadership-class computing resources. The ALCF's Aurora Early Science Program also supports 10 projects focused on employing data and learning on the facility's upcoming exascale supercomputer. In addition, DOE's INCITE program has expanded its focus beyond traditional simulation-based projects to support research campaigns that involve data science and machine learning applications.

The ALCF's supercomputing resources are also pushing the facility's evolution to a more data-centric research center. In 2020, the ALCF augmented its Theta supercomputer with graphic processing units (GPU) to provide a new resource, known as ThetaGPU, that can integrate data analytics with AI training and learning workloads. With Polaris and Aurora on the horizon, the ALCF will continue to add GPU-accelerated machines that are built to handle data-intensive computing.

To maximize the capabilities of these systems, ALCF staff members play a key role in ensuring the machines are equipped with software stacks that support performant, scalable data science and machine learning frameworks, workflow packages, Jupyter notebooks, containers, and more. This includes custom-built software tools designed for specific tasks, as well as open-source software tools adapted to meet various research needs.

In addition to providing resources to enable data-driven discoveries, the ALCF's evolving suite of services and tools aims to help to eliminate barriers to productive use of the facility's systems; integrate with user workflows to produce seamless, usable environments; and enhance collaboration among research teams. The facility's growing collection of data science resources and expertise is creating a hub for storing, sharing, analyzing, and reusing data that will ultimately help accelerate the pace of discovery.

Integrating the ALCF with experimental facilities

The ALCF's new supercomputing resource gives researchers a testbed to prepare scientific applications and workloads for Aurora.

Data science, always a fundamental part of leadership computing, is now driving a convergence of high-performance computing (HPC) and laboratory sciences as experimental facilities upgrade their instruments and capabilities parallel to the emergence of the exascale era. While state-of-the-art experimental facilities will be able to generate orders of magnitude more data than even their most powerful predecessors, their computational demands grow commensurately.

To test and push the limits of integrating HPC and experimental facilities, the ALCF recently acquired four additional racks of nodes for its newest leadership computing system, Polaris.

The Polaris expansion, which augments the system's capacity for computational tasks in general, helps drive experimental integration by presenting opportunities for increased collaboration with critical resources and facilities such as Argonne National Laboratory's Advanced Photon Source (APS), the Center for Nanoscale Materials (CNM), and ATLAS.

The steepening computational requirements of next-generation experimental facilities like the APS-U make exclusive reliance on local computing systems increasingly impractical. On-the-fly, real-time processing is now crucial for analyzing the data produced by the facilities' instruments. Coupling this with increasingly multifaceted analysis methods, such as AI-driven machine learning algorithms integrated into complex workflows, solidifies the need for tighter integration of HPC and experimental facilities.

The Polaris expansion promises to make large-scale data processing a more seamless experience, enabling users to begin processing data while experimental instruments are still in operation—and even before all data have been transferred—opening up new avenues for powerful machine learning methods and real-time insights into the experiment.

Moreover, integrating experimental facilities and the ALCF establishes a relationship whereby each facility is well-positioned to serve the other. An ALCF user will be able to retrieve data on the fly from the APS or CNM just as easily as an APS or CNM user could refer to ALCF resources for a calculation.

The integration requires the ALCF to address both social and technical challenges. Principal among these is reconciling with experimentalists' need for immediate data analysis the traditional HPC means of operating through batch modes that submit jobs to a queue to run as computational resources become available. Technical work is underway to test preemptive scheduling queues that provide the ability to stream data from APS detectors directly to the Polaris system. Work is underway to help develop community understanding of preemption, as is social engineering to encourage user adoption of preemptable queues.

The colocation of the ALCF and the Advanced Photon Source (APS) at Argonne National Laboratory offers a unique opportunity to develop and demonstrate a model for tightly coupling experiments and supercomputing facilities.

Other challenges to HPC-experimental integration include:

Aligning maintenance schedules at integrated facilities to minimize interruptions
Maintenance schedules vary from facility to facility. The APS runs, for instance, for approximately two months prior to an extended outage, whereas the ALCF undergoes maintenance every two weeks for eight to twelve hours.

Security
The ALCF requires two-factor authentication, a manual process that must be reconciled with the goal of fully automating APS analysis workflows.

Sharing nodes
The ALCF historically has not allowed users to share nodes but is revisiting that stance given the new capabilities of both hardware and software. Shared nodes have the potential to enable more efficient and productive allocations, and doing so presents technical, security, and reporting issues that must first be resolved.

Polaris to help pave the way to exascale

The ALCF's new supercomputing resource gives researchers a platform to prepare scientific applications and workloads for Aurora.

With the arrival of the Polaris supercomputer at the ALCF, researchers will have a powerful new tool to prepare for science in the exascale era.

Developed in collaboration with Hewlett Packard Enterprise (HPE), Polaris is a leading-edge system that will give scientists and application developers a platform to test and optimize codes for Aurora, the ALCF's upcoming Intel-HPE exascale supercomputer. Like Aurora, Polaris is a hybrid system equipped with both graphics processing units (GPUs) and central processing units (CPUs).

Aurora, along with DOE's other next-generation exascale machines, will combine unprecedented processing power with advanced capabilities for artificial intelligence (AI) and data analysis, enabling researchers to tackle important scientific challenges, such as discovering new materials for clean energy applications, increasing our understanding of the global impacts of climate change, and exploring the increasingly large datasets generated at DOE experimental facilities, at a scale not possible today.

But conducting science on machines that are orders of magnitude more powerful than today's top supercomputers requires significant preparatory work. With DOE's Exascale Computing Project (ECP) and initiatives like the ALCF's Aurora Early Science Program, researchers have been working behind the scenes for years to ensure applications, software, and hardware will be ready for science as soon as the first exascale systems are deployed. Polaris, the ALCF's largest GPU-accelerated system to date, will be a valuable resource for Argonne researchers and the entire scientific community as they continue to prepare for DOE's forthcoming exascale machines.

The HPE Apollo Gen10+ based supercomputer is equipped with 560 AMD EPYC processors and 2,240 NVIDIA A100 Tensor Core GPUs. The system will deliver approximately 44 petaflops of peak double precision performance and nearly 1.4 exaflops of theoretical artificial intelligence (AI) performance, which is based on mixed-precision compute capabilities. Like Aurora, Polaris uses the Slingshot interconnect technology, which is designed to support the simulation, data, and machine learning workloads that will drive science in the exascale era.

The Polaris software environment features the HPE Cray programming environment, HPE Performance Cluster Manager (HPCM) system software, and the ability to test programming models—such as OpenMP and SYCL—that will be available on Aurora and the next-generation supercomputers at the OLCF and NERSC. Polaris users will also benefit from NVIDIA's HPC software development kit, a suite of compilers, libraries, and tools for GPU code development.

Polaris is a hybrid CPU-GPU system built by HPE.

The delivery and installation of Polaris began in August 2021. Initially, the system will be dedicated to research teams participating in the ECP, Aurora Early Science Program, and the ALCF Data Science Program. In 2022, Polaris will be made available to the broader HPC community for a wide range of science and engineering projects, including some INCITE awards.

In addition to helping pave the way to exascale, Polaris is a key resource for expanding the ALCF's scope beyond that of a traditional high-performance computing facility. With architectural features that support AI and data-centric workloads, Polaris is particularly well-suited to handle the massive amounts of data being produced by large-scale simulations and experimental facilities. Initial efforts will be focused on integrating HPC and AI workloads with experimental facilities located at Argonne, including the Advanced Photon Source and the Center for Nanoscale Materials.

With many similarities at the system and user levels, Polaris will be a key resource for researchers preparing to use the ALCF's Aurora exascale supercomputer.

SYSTEM NAME	POLARIS
System Software	HPCM
Programming Models	MPI, OpenMP, DPC++, Kokkos, RAJA, HIP, CUDA, OpenACC
Tools	CrayPat, gdb, Cray ATP, NVIDIA Nsight, cuda-gdb
MPI	CrayMPI, MPICH
Multi-GPU	1 CPU : 4 GPU
Data and Learning	DL frameworks, Cray AI stack, Python/Numba, Spark, Containers, Rapids
Math Libraries	cu* from CUDA

SYSTEM NAME	AURORA
System Software	HPCM
Programming Models	MPI, OpenMP, DPC++, Kokkos, RAJA, HIP
Tools	CrayPat, gdb, Cray ATP, Intel VTune
MPI	CrayMPI, MPICH, Intel MPI
Multi-GPU	2 CPU : 6 GPU
Data and Learning	DL frameworks, Cray AI stack, Python/Numba, Spark, Containers, oneDAL
Math Libraries	oneAPI

Shared features are shown in white.

The Road to Aurora

Behind the scenes, ALCF staff members and exascale application development teams are working to ensure Aurora is ready for science on day one.

Standing up a first-of-its-kind exascale supercomputer is a massive undertaking that requires ingenuity, diligence, and collaboration. While the sheer computational power of future exascale systems may grab the headlines, the behind-the-scenes work to prepare for their arrival continues to be a momentous feat.

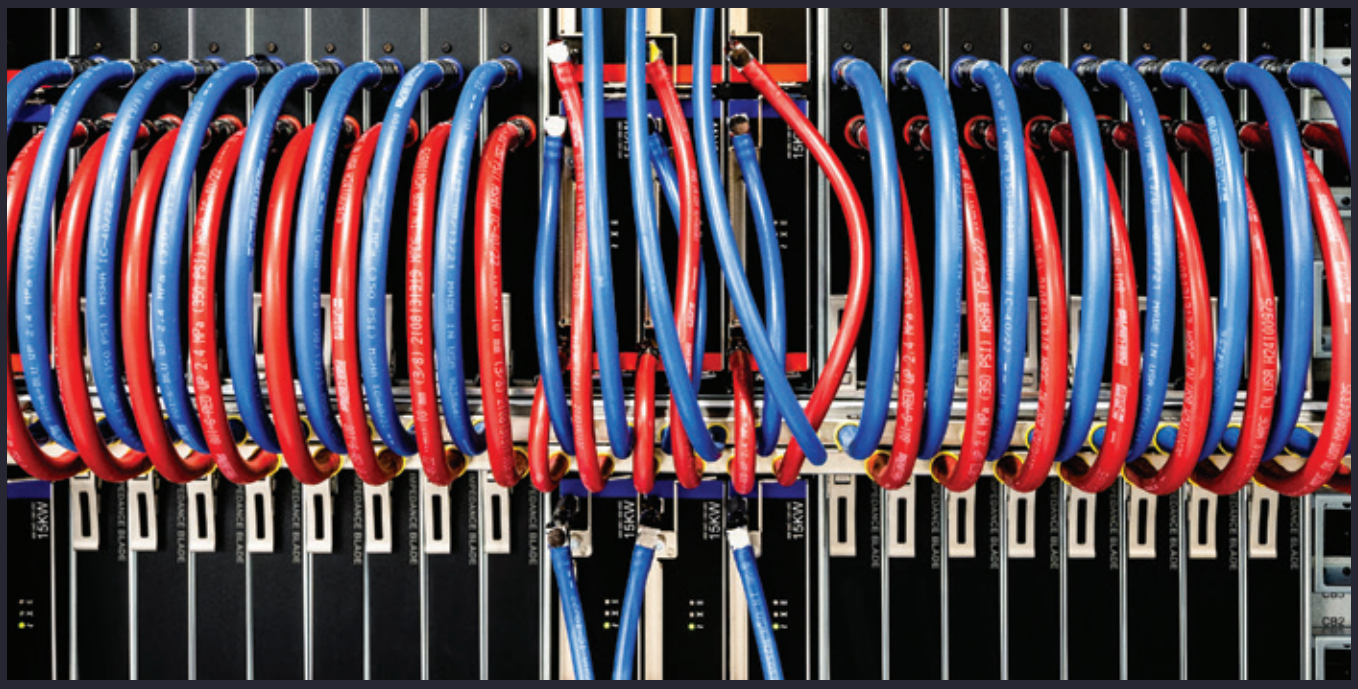
With the delivery of Aurora, an Intel-Hewlett Packard Enterprise (HPE) supercomputer, drawing closer, a dedicated team of ALCF staff members has been working to ensure hardware, software, and a diverse set of scientific computing applications are ready for the research community as soon as the system is deployed for science.

The team's work covers everything from exascale code development and hardware technology evaluations to user training and close partnerships with vendors, fellow national laboratories, and DOE's Exascale Computing Project (ECP).

These activities and collaborations are laying the groundwork for Aurora to drive a new era of scientific discoveries and technological innovations at the ALCF and beyond.

Aurora Architecture

Aurora's innovative design will be based on Intel's Xeon Scalable processors, high-performance Intel X^{e} GPU compute accelerators, and Optane DC persistent memory. The system will rely on HPE Cray EX architecture and HPE Slingshot technology, which can provide concurrent support for advanced simulation and modeling, AI, and analytics workflows. Aurora will leverage historical advances in software investments along with increased application portability via Intel's oneAPI. The supercomputer will also be equipped with a new I/O platform called Distributed Asynchronous Object Storage (DAOS) to meet the needs of exascale workloads.



Aurora's cooling infrastructure will pump 44,000 gallons of water through the system.

Peak Performance

>2 Exaflops DP

Platform

HPE Cray EX

GPU

Intel Xe arch-based "Ponte Vecchio" GPUs

CPU

Intel Xeon scalable "Sapphire Rapids" processors

Compute Node
2 Intel Xeon scalable "Sapphire Rapids" processors; 6 Xe arch-based GPUs; Unified Memory Architecture; 8 fabric endpoints; RAMBO

GPU Architecture
Xe arch-based "Ponte Vecchio" GPU; Tile-based chiplets, HBM stack, Foveros 3D integration, 7nm

CPU-GPU Interconnect
CPU-GPU: PCIe
GPU-GPU: Xe Link

System Interconnect
HPE Slingshot 11; Dragonfly topology with adaptive routing

Network Switch
25.6 Tb/s per switch, from 64–200 Gbs ports (25 GB/s per direction)

High-Performance Storage
≥230 PB, ≥25 TB/s (DAOS)

Programming Models
Intel oneAPI, MPI, OpenMP, C/C++, Fortran, SYCL/DPC++

Node Performance
>130 TF

Aggregate System Memory
>10 PB

System Size
>10,000 nodes

Exascale Expertise

ALCF's Brice Videau is working to maximize the portability of HIP applications for exascale systems.

The process of planning and preparing for a new leadership-class supercomputer takes years of collaboration and coordination. It requires partnerships with vendors and the broader HPC community to test and develop various hardware and software components, validating their performance and functionality meets the needs of the scientific computing community.

The following summaries provide a look at a few of the many ALCF staff efforts underway to ready the facility and its users for the exascale computing era.

HIPLZ

Brice Videau, a computer scientist at ALCF with years of experience in code generation, optimization, and auto-tuning high-performance computing, is leading efforts to maximize the portability of HIP applications being developed for the next generation of leadership computing systems, including Argonne's forthcoming exascale Aurora system.

Already established as the default programming model for AMD GPUs, many prominent applications are expected to adopt HIP as a programming model as they target deployment on upcoming exascale systems. Furthermore, HIP provides support for NVIDIA platforms, enabling HIP application portability across AMD and NVIDIA hardware. With HIP a likely programming model for numerous exascale codes, Videau's team wants to ensure that HIP applications are as portable as possible.

The HIPLZ project, to this end, aims to investigate the best way to enable native support for HIP applications on Aurora. Videau's team ultimately leverages Level Zero, a new API that Intel is developing for its GPUs, including the Ponte Vecchio accelerators that will drive Aurora.

As part of the team's development strategy, Videau and colleagues are building on the work of an earlier project that developed HIPCL, a library which enables HIP to run on top of OpenCL. Because Aurora will feature Level Zero as its primary low-level GPU interface, HIPLZ redirects the efforts of HIPCL in order to facilitate support for HIP applications on Level Zero.

ALCF's Kris Rowe (left) and Saumil Patel are working to bring the open-source OCCA library to Aurora.

ALCF's Corey Adams is helping to ensure deep learning frameworks are ready for Aurora.

The OCCA Library

ALCF computational scientist Kris Rowe is leading collaborative efforts to bring OCCA—an open-source, vendor-neutral framework and library for parallel programming on diverse architectures—to Aurora.

Mission-critical computational science and engineering applications from the DOE and private industry rely on OCCA, which provides developers with transparency in the generation of raw backend code. NekRS, for example—a new computational fluid dynamics solver from the Nek5000 developers—is used simulate coolant flow inside of small modular reactors and design more efficient combustion engines.

Utilizing OpenMP and DPC++, Rowe worked with Saumil Patel of Argonne's Computational Sciences Division to establish initial benchmarks for various types of kernels before beginning development of the SYCL/DPC++ OCCA backend. Rowe and Patel meet biweekly with an Intel team to coordinate testing and performance aspects, and to drive the development of new features.

Programming models used by the OCCA backends continually evolve. Rowe currently surveys the latest DPC++, OpenMP, CUDA, and HIP specifications to identify common performance critical features—such as asynchronous memory transfers and work-group collectives—which have yet to propagate into the OCCA. Using this information, the team will propose extensions to the existing OCCA API for inclusion in future releases of the framework.

Deep Learning Frameworks

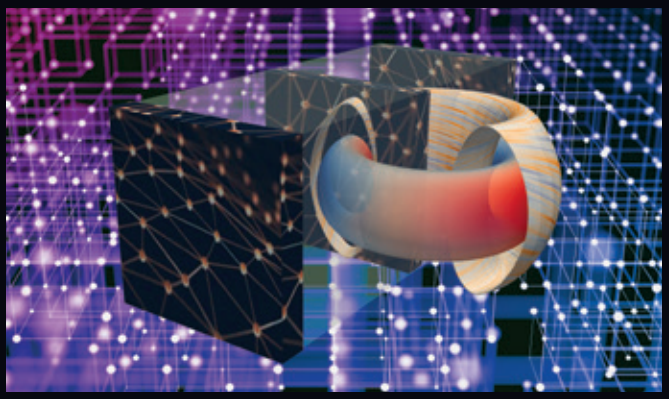
ALCF computer scientist Corey Adams is leading efforts to deploy advanced deep learning frameworks on Aurora, ensuring that key applications are fully performant on Day 1—that they run well and scale well in relatively bug-free implementations.

To this end, Corey and his colleagues selected a number of Argonne workloads that represent innovative AI-for-science approaches that will benefit from the Aurora architecture. In doing so, in order to grow application capabilities from a science perspective, they built on computer vision benchmarks established by Intel during the development of various deep learning and AI frameworks.

High-level frameworks in Python, such as TensorFlow and PyTorch, rely on Intel's deep neural network (DNN) framework oneDNN for computationally intensive GPU processes such as convolution operations, the complex demands of which frustrate attempts at out-of-the-box performance. This necessitates extensive iterations of development and testing before an efficient kernel or source code can be produced.

Once optimal performance has been achieved on a single GPU, the Intel Collective Communications Library oneCCL helps deliver optimal performance on multiple GPUs by distributing optimized communications patterns to allocate parallel model training among arbitrarily many nodes. OneCCL and the synchronicity it encourages thereby enable tasks such as the uniform collection of gradients from a training iteration.

Programming for Aurora



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

Through the DOE's Exascale Computing Project and the ALCF's Aurora Early Science Program, research teams across the country are working to prepare applications to run efficiently on the ALCF's upcoming exascale system. With access to the early exascale hardware and Aurora SDK, researchers are porting various codes, mini-apps, frameworks, and libraries to evaluate and optimize their performance using the programming models that will be supported on Aurora. The following summaries provide a look at a handful of the many exascale application development efforts currently underway.

Fusion Energy Research

Princeton Plasma Physics Laboratory is leading a project that uses artificial intelligence methods to improve predictive capabilities and mitigate large-scale disruptions in burning plasmas in tokamak systems such as ITER.

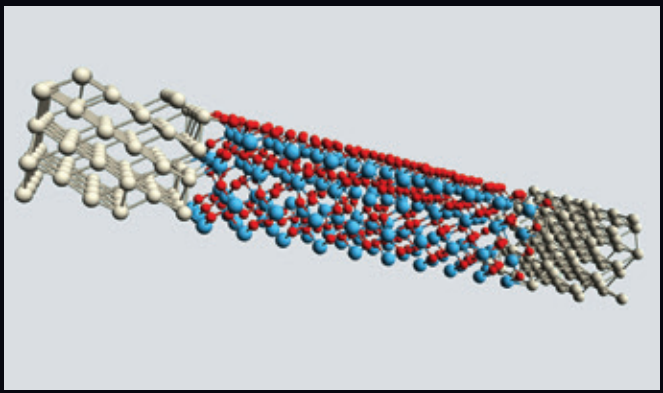
ALCF staff are working to port the project's primary application, the FusionDL FRNN (Fusion Recurrent Neural Net) suite, to Aurora, which stands to enable fusion researchers to train increasingly large-scale deep learning models able to predict with greater accuracy the onset of plasma instabilities in tokamak reactors. The increased processing and predictive powers of exascale will permit more exhaustive hyperparameter tuning campaigns that in turn can lead to better-optimized configurations for the AI models.

The developers aim to accelerate and improve communications between experimental sites and the supercomputing facilities with which they interact; the turnaround times for data transfers and for training new model architectures are expected to shorten significantly.

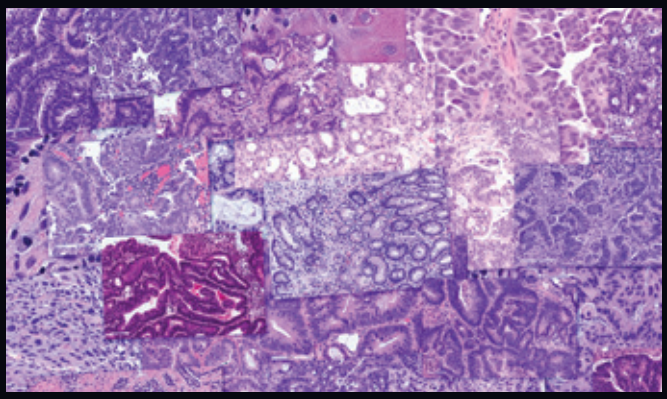
Collaborating with Intel engineers to diagnose the causes of model underperformance relative to NVIDIA capabilities has helped the development team more deeply understand their models. The team has evaluated and profiled their software on NVIDIA systems, ThetaGPU's A100s, via Nsight Systems software. The insights gleaned will help inform and calibrate expectations on Polaris and on Intel GPUs in preparation for Aurora.

QMCPACK

Quantum Monte Carlo (QMC) methods are ideal candidates for the next generation of material-design tools, which target not only simple bulk properties but collective effects in strongly correlated materials. The open-source QMCPACK



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



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

simulation code performs electronic structure calculations via accurate approximation of the Schrodinger equation. Run on all DOE supercomputers, it has been used for research at the ALCF since 2011.

A multi-institutional effort is now underway to prepare QMCPACK for deployment on forthcoming, GPU-powered exascale machines, including the Aurora supercomputer. The greatly expanded computational power and parallelism of exascale will enable predictive capabilities far beyond the capacity of QMCPACK's current implementation.

To facilitate a variety of vendor-specific libraries, the developers are redesigning the entire infrastructure of QMCPACK. The intent is to ensure there exists a general framework that enables the flexible implementation of higher-level algorithms while allowing specialized implementations to run at a lower level as needed.

The exascale port of QMCPACK has been deployed for production science on leadership machines including the ALCF's Theta and the Oak Ridge Leadership Computing Facility's Summit; the developers continue to consolidate QMCPACK for optimal performance on Intel and AMD hardware.

In attempting to attain optimal performance, the developers take a holistic approach that accounts for the entirety of their software stack and hardware. In addition to creating fast compute kernels, the developers focus on minimizing resource idle on host processors.

CANDLE

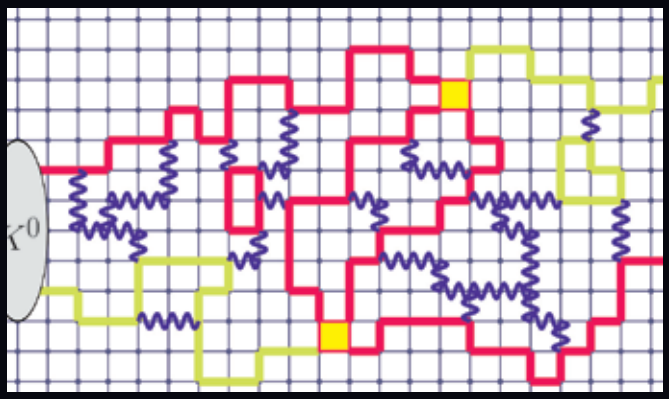
Developed as part of the ECP's Exascale Deep Learning and Simulation Enabled Precision Medicine for Cancer project, CANDLE (or the CANcer Distributed Learning Environment), is an exascale-optimized framework that seeks to leverage the next generation of supercomputing to answer broad questions cancer researchers face.

CANDLE will be deployed on DOE supercomputers such as the forthcoming Aurora system. The software suite broadly consists of three components: a collection of deep neural networks that capture and represent different problems in cancer, a library of code adapted for exascale-level computing, and a component that orchestrates how work will be distributed across the computing system.

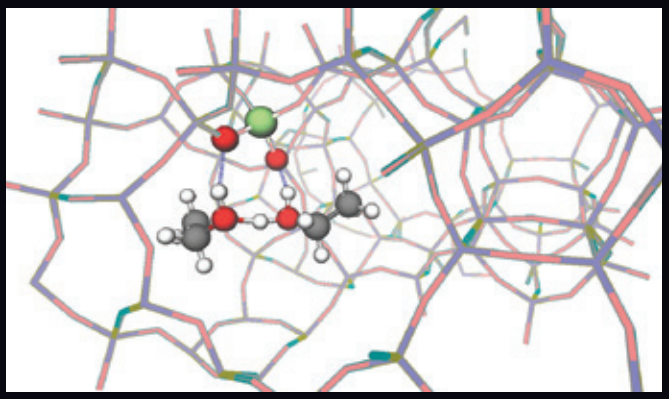
The project seeks to implement deep learning architectures both relevant to cancer research and capable of addressing critical problems therein at three biological scales: cellular, molecular, and population-level.

While the application is hardware-agnostic, its particular implementation relies on the deep learning framework. This means that while the code will run on Aurora and other DOE supercomputers alike, its implementations may vary if two given machines incorporate different frameworks. Differences in the underlying hardware (for example, an Intel GPU versus an NVIDIA GPU), meanwhile, may lead to the presence of various custom-tuning techniques.

Machine learning and deep learning-based applications such as CANDLE can only be successfully ported subsequent to the successful implementation of their underlying software framework—an ecosystem like Python, TensorFlow, PyTorch, or Keras. Successful implementation occurs in a two-step process. First the functionality of the application must be tested—that is, the code must successfully execute in full in a limited setting without incurring any serious bugs. The software framework implementation requires further optimization to help the application satisfy the convergence criteria with maximum performance metrics, such as throughput.



A schematic representation of a Lattice QCD calculation of the one part per 100 trillion difference in mass between the long- and short-lived K mesons. ***Image: Norman Christ, Columbia University***



NWChemEx is based on NWChem, an open-source, high-performance parallel computational chemistry code. ***Image: NWChemEx Team***

LATTICE QCD

The fundamental interactions between the quarks and gluons that constitute protons and nuclei can be calculated systematically by the physics theory known as lattice quantum chromodynamics (LQCD). These interactions account for 99 percent of the mass in the visible universe, but they can only be simulated with powerful leadership computer systems.

Exascale capabilities promise to expand high energy and nuclear physics by providing the ability to simulate atomic nuclei more realistically than has ever been possible, enabling groundbreaking discoveries about the details of quark-boson coupling foundational to our present understanding of elementary particles.

The LQCD application suite's three major code bases specialize in different quark discretizations and take advantage of optimized routines available in the QUDA ("QCD in CUDA") library and Grid code. The project additionally supports two minor code bases, HotQCD, which is optimized for QCD thermodynamics, and QEX, which is intended for high-level development of lattice field theory codes.

Abstraction is the primary thrust of the porting process; the developers are working to make all the performance critical parts of the LQCD codes completely vendor-independent. The changes made through the abstraction process are localized to a few backend files that provide functionality for mathematical operations. Once all of these backend and target-specific calls are grouped, they can be replaced or rewritten with higher-level functions that make the code more generic.

The developers must also determine how to make an OpenMP thread that maps to CPU cores compatible with GPUs. As with the majority of CPUs, all GPUs are SIMD machines. This means that on a CPU machine a CPU thread would execute a vector instruction and that on a GPU machine a GPU thread would execute a vector instruction.

NWCHEMEX

NWChem is a widely used, open-source computational chemistry package. With the NWChemEx project supported by ECP and the Aurora ESP, a multi-institutional team is working to redesign and reimplement the software package to provide a next-generation molecular modeling package for exascale.

This effort has provided the opportunity to restructure core functionality—including the elimination of longstanding bottlenecks associated with the generally successful NWChem code—concurrent with the production of sophisticated physics models intended to leverage the upcoming exascale systems. The development team is using multiple programming models, including CUDA, HIP, and DPC++ to maximize flexibility and target various hardware accelerators.

To help localize communication and thereby reduce related bottlenecks, NWChemEx is being geared such that CPUs handle communication protocols as well as any other non-intensive components (that is conditional-structure-based algorithms). Anything else—anything "embarrassingly parallel" or computationally expensive—is to be processed by GPUs.

In order to understand the degree to which the application is utilizing experimental hardware, the developers implement a multitiered analysis for tracking code performance. They then conduct a postmortem analysis to pinpoint the origin of errors and establish the scope of improvement that theoretically can be expected.

Aurora Hackathons and Dungeon Sessions*

02/08
Simulating and Learning in the ATLAS Detector at the Exascale

03/05, 09/16, 10/14
Kokkos Hackathon

05/20–05/21
Extreme-Scale Unstructured Adaptive CFD

05/27
Aurora Mini-Dungeon (focused on Fortran)

06/15–06/17
Aurora Dungeon 2 (LQCD, XGC, RxMD/QxMD, NAMD)

09/23
Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

12/13–12/14
Virtual Drug Response Prediction

12/16
Accelerated Deep Learning Discovery in Fusion Energy Science

**Supported by the Argonne-Intel Center of Excellence*

Aurora Webinars

03/24
SYCL 2020 & DPC++: Improvements to the SYCL Programming Model

06/30
Performance, Portability, and Productivity

09/29
Preparing Applications for Aurora: OpenACC to OpenMP Migration Tool

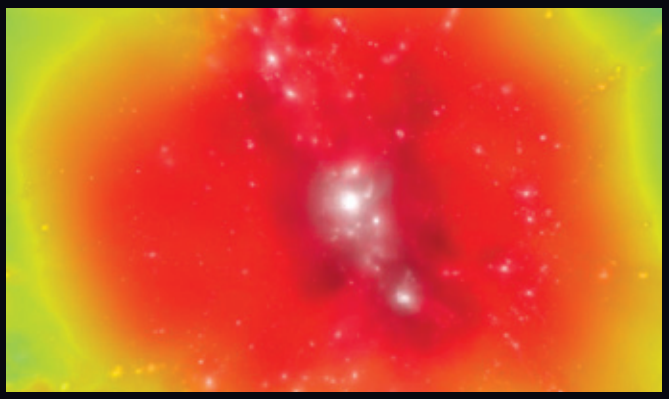
12/17
Reduce Cross-platform Programming Effort and Write Performant Parallel Code with oneDPL

Aurora Workshop

10/26–10/27, 12/7–12/9
Aurora COE Workshop 2: Aurora Software Development Kit and Hardware Overview

Aurora Early Science Program Projects

Simulation Projects



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

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

The program is supporting five simulation projects, five data projects, and five learning projects. The diverse set of projects reflects the ALCF's effort to create an environment that supports emerging data science and machine learning approaches alongside traditional modeling and simulation-based research.

Extending Moore's Law Computing with Quantum Monte Carlo

PI Anouar Benali
INST Argonne National Laboratory

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang
INST Princeton Plasma Physics Laboratory

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

PI Theresa Windus
INST Iowa State University and Ames Laboratory

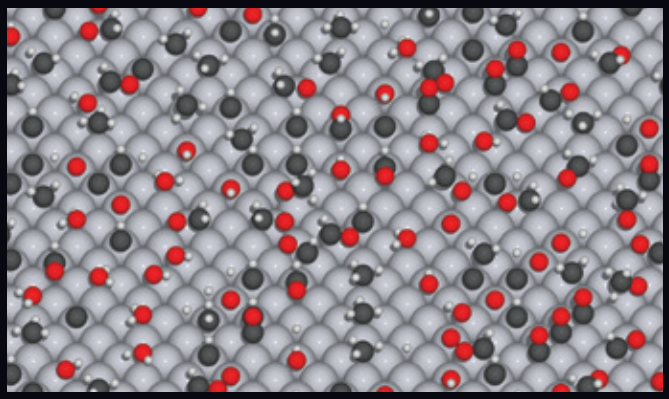
Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann
INST Argonne National Laboratory

Extreme-Scale Unstructured Adaptive CFD

PI Ken Jansen
INST University of Colorado Boulder

Data Projects



The Exascale Computational Catalysis project will combine data science techniques and quantum chemistry simulations to explore the otherwise intractable phase space resulting from gas phase molecules on catalyst surfaces to find relevant configurations and the lowest transition states between them. *Image: Eric Hermes, Sandia National Laboratories*

Exascale Computational Catalysis

PI David Bross
INST Argonne National Laboratory

Dark Sky Mining

PI Salman Habib
INST Argonne National Laboratory

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI Ken Jansen
INST University of Colorado Boulder

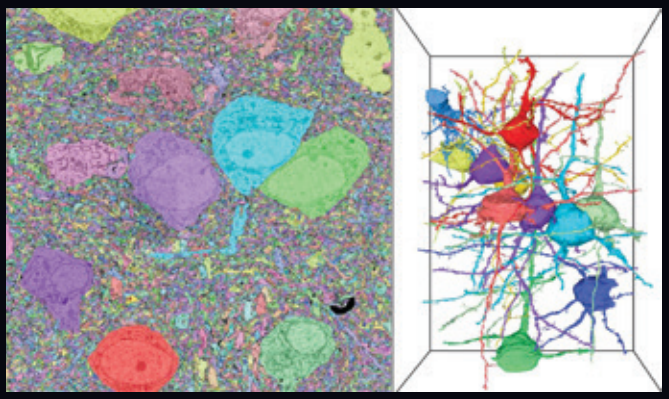
Simulating and Learning in the ATLAS Detector at the Exascale

PI Walter Hopkins
INST Argonne National Laboratory

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

PI Amanda Randles
INST Duke University and Oak Ridge National Laboratory

Learning Projects



Left: Data from electron microscopy; grayscale with color regions showing segmentation. Right: Resulting 3D representation. *Image: Nicola Ferrier, Tom Uram and Rafael Vescovi, Argonne National Laboratory; Hanyu Li and Bobby Kasthuri,University of Chicago*

Machine Learning for Lattice Quantum Chromodynamics

PI William Detmold
INST Massachusetts Institute of Technology

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI Nicola Ferrier
INST Argonne National Laboratory

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

PI Noa Marom
INST Carnegie Mellon University

Virtual Drug Response Prediction

PI Rick Stevens
INST Argonne National Laboratory

Accelerated Deep Learning Discovery in Fusion Energy Science

PI William Tang
INST Princeton Plasma Physics Laboratory

GROWING THE HPC COMMUNITY

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

Argonne hosts and contributes to a number of events designed to share the latest advances in scientific computing.

Creating a Diverse and Inclusive Workplace

The ALCF is committed to building a culture that supports and celebrates diversity, equity, and inclusion.

As a world-class computing facility, the ALCF strives to recruit, hire, and retain the very best people—a diverse group of smart, talented, and capable men and women who are committed to our mission of providing supercomputing resources and expertise to enable new scientific discoveries and innovations.

The ALCF's goal is to build a diverse team whose cultural and intellectual backgrounds equip the facility to look at problems from a variety of viewpoints, resulting in creative solutions to complex challenges in scientific computing. While there is much work to be done, the facility remains committed to making diversity, equity, and inclusion (DEI) an inherent part of the ALCF workplace and culture.

From organizing camps to inspire the next generation of computing experts to driving Argonne initiatives that promote diversity across the laboratory, ALCF staff members are involved in many activities aimed at fostering a world-class, 21st-century workplace.

Supporting Diversity Across Argonne

Active in Argonne employee research groups (ERGs) for women, LGBTQIA+ employees, and African Americans, ALCF staff are helping to build awareness, further personal and professional development, strengthen networking opportunities, and provide resources for laboratory employees.

Argonne's Argonne African American Employee Resource Group (AAA-ERG) partners with laboratory leadership to promote the development of African Americans in science, technology, and operations. ALCF Director Michael Papka serves as an executive sponsor for AAA-ERG, helping to support the group's mission to foster an inclusive, collaborative workplace for all Argonne employees, and develop a pipeline for future talent at the laboratory through scholarships, educational programs, networking and cultural events.

ALCF staff members have been integral to the creation and operation of Spectrum, an Argonne ERG dedicated to building awareness and providing resources for those in the laboratory community who identify as lesbian, gay, bisexual, transgender, queer, questioning, intersex, asexual, agender, or allies to their LGBTQIA+ peers. ALCF's Skip Reddy was a co-founder of the group. ALCF's Carissa Holohan continues to serve as a co-leader of the organization, helping to promote a welcoming and inclusive work environment, advise the laboratory on employee issues, advance LGBTQIA+ friendly policies and benefits, and participate in outreach and talent recruitment activities.

Argonne's Women in Science and Technology (WIST) program is a dynamic community of science and technology professionals that provides support, guidance, and professional development to women at the laboratory.

Argonne's annual computing camps provide students with an opportunity to explore potential careers in STEM.

WIST works to recruit, retain, and promote women for greater diversity and strength in the laboratory's scientific workforce. The ALCF's Jini Ramprakash, Yasaman Ghadar, and Avanthi Mantrala serve on the steering committee helping to provide a well-rounded perspective on the approach to achieving its mission of equal education and awareness of STEM opportunities, and support and mentorship to women pursuing careers in STEM.

Introducing Girls to STEM Careers

Educational and outreach programs, including summer camps and internship opportunities, also help introduce students and early-career scientists and engineers to the mission-driven, high-impact research conducted at Argonne and beyond.

Through participation in Argonne's annual Introduce a Girl to Engineering Day (IGED) and Science Careers in Search of Women (SCSW) events, ALCF staff members have the opportunity to connect with young women and introduce them to potential career paths in science, technology, engineering, and mathematics (STEM). IGED pairs approximately 100 local eighth graders with Argonne engineers and scientists for a day of presentations and hands-on activities focused on STEM careers. SCSW hosts high school students for a day of STEM activities, including Q&A panel discussions with Argonne women scientists, facility tours, and a career fair.

Taught by ALCF computing researchers and staff from the lab's Learning Center, the annual CodeGirls@Argonne Camp hosts sixth and seventh-grade girls each summer for a three-day event dedicated to teaching them the fundamentals of coding. The virtual camp gave students an opportunity to try out creative and computational thinking through activities that include programming robots. The camp also allowed participants to meet women

Facility tours give students a firsthand look at the role supercomputers play in scientific research.

scientists, who use code to solve problems, and take part in a virtual tour the ALCF's machine room and visualization lab.

Building a diverse team and community
As part of the ALCF's efforts to cultivate a diverse and talented workforce, the facility has a presence at many computing conferences and events to recruit new team members.

The annual Grace Hopper Celebration (GHC) brings the research and career interests of women in computing to the forefront, and highlights the contributions of women to the tech world. GHC has become the world's largest gathering of women technologists, where women from around the world learn, network, and celebrate their achievements. ALCF has had a presence at the GHC event and career fair for several years, including a virtual booth at GHC 2021.

The annual Richard Tapia Celebration of Diversity in Computing Conference seeks to bring together undergraduate and graduate students, faculty, researchers, and professionals in computing from all backgrounds and ethnicities to celebrate and connect the diversity in computing. Several ALCF staff members gave presentations at this year's event, providing tutorials and materials designed to help attendees gain deeper knowledge of HPC.

The Broader Engagement program at the Society of Industrial and Applied Mathematics' (SIAM) 2021 Computational Science and Engineering (CSE21) conference provided a rich scientific program, mentoring, and career and professional development to students from underrepresented and underprivileged backgrounds who aspire to broaden their experience in research-based professional activities. Serving on the Broader Engagament program's organizing committee, the ALCF's Jini Ramprakash helped plan outreach activities and chaired the program's poster session at CSE21.

In addition to recruiting new staff members, the ALCF also aims to increase diversity in its user community through an ongoing partnership with the Interdisciplinary Consortium for Research and Educational Access in Science and Engineering (InCREASE), a group dedicated to promoting research and education in minority-serving institutions. As part of the InCREASE partnership, the ALCF participates in user facilities awareness workshops aimed at building new research collaborations with scientists from historically underrepresented groups.

Partnering with Industry

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

Focused on growing the facility's community of industry users, the ALCF's Industry Partnerships Program engages with prospective companies of all sizes, from start-ups to Fortune 500 corporations, that could benefit from leadership computing resources and collaborative opportunities with the ALCF and across Argonne.

The ALCF's leadership computing resources—equipped with advanced simulation, data, and learning capabilities—enable companies to tackle problems that are too computationally demanding for traditional computing clusters.

Access to ALCF systems and expertise allows industry researchers to make predictions with greater accuracy, rapidly analyze massive datasets, and create higher-fidelity models of everything from manufacturing processes to fusion energy devices. The results permit companies to accelerate critical breakthroughs, verify uncertainties, and drastically reduce or eliminate the need to build multiple prototypes.

The ALCF has enhanced its industry outreach program by partnering with other Argonne user facilities and divisions, including the Technology Commercialization and Partnerships Division. By providing more complete picture of the laboratory's resources, this collaborative approach has resulted in broader engagements across Argonne with a number of companies.

The ALCF is also actively involved in directing the DOE Exascale Computing Project's Industry and Agency Council, an advisory group of senior executives from prominent U.S. companies and U.S. government agencies interested in working with Argonne and other DOE laboratories to deploy exascale computing to improve their products and services.

DRIVING INNOVATION FOR INDUSTRY

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

Advancing Fusion Energy Research

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

Improving the Energy Efficiency of Jet Engines

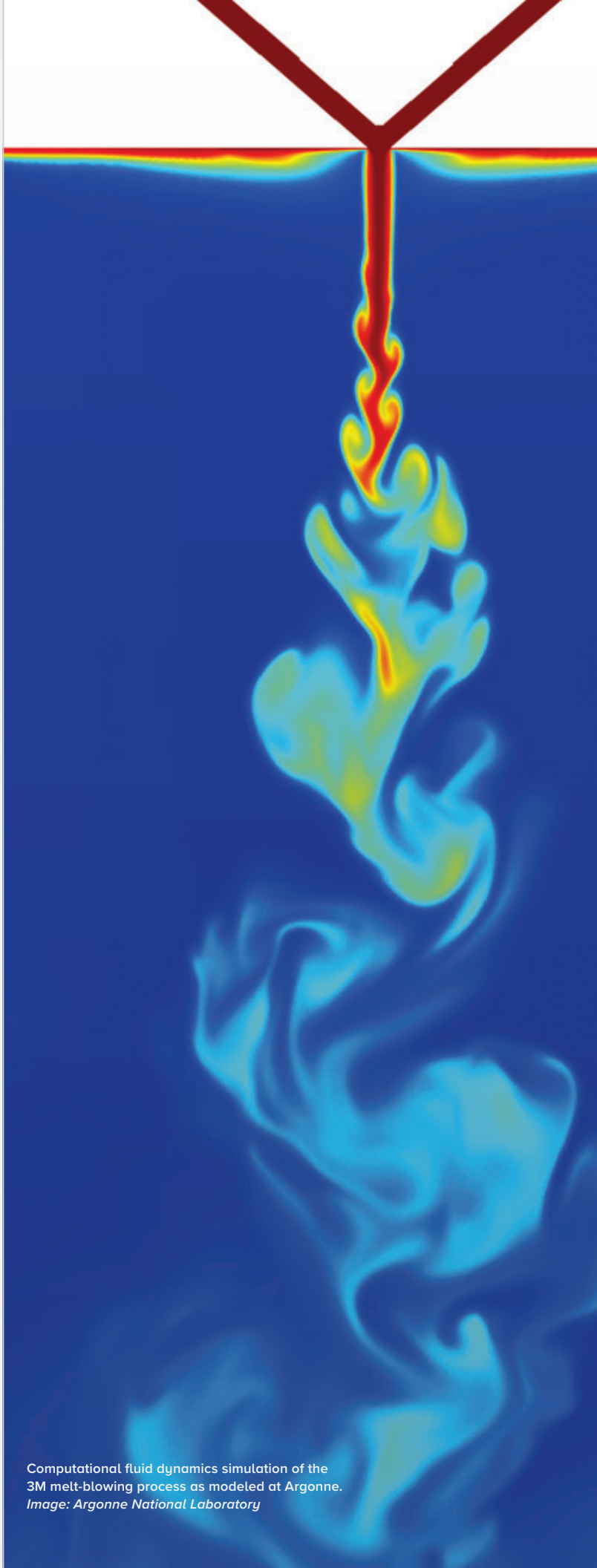
Argonne is once again partnering with Raytheon Technologies Research Center to use machine learning to improve the performance, design, and energy efficiency of gas turbine engines. This project will use complex modeling to better quantify the impact of manufacturing uncertainties on the energy efficiency of Raytheon's jet engines.

Reducing Energy Consumption in Fiber Manufacturing

Working with 3M Co., Argonne is using HPC, fluid-dynamics simulations, and machine learning to minimize the energy used in the melt-blown fiber manufacturing process. This extremely energy-intensive process is widely used by 3M to produce filters, fabrics, and insulation materials, as well as the N95 mask used for protection during the COVID-19 pandemic. By improving this manufacturing process, engineers can reduce the energy consumed by 20%, which would save the industry nearly 50 gigawatt hours per year.

First-Ever DNS of a Full-Scale Modern Automotive Engine

Researchers from Argonne performed direct numerical simulation of flow in a full-scale, modern automotive engine using an INCITE 2021 allocation. The simulation data is being used to develop improved wall heat transfer models, which will help automotive OEMs to perform numerical optimization of engine designs to improve efficiency and reduce emissions.



Computational fluid dynamics simulation of the 3M melt-blowing process as modeled at Argonne.
Image: Argonne National Laboratory

Shaping the Future of Supercomputing

ALCF researchers participate in numerous activities that aim to advance the forefront of scientific computing.

As a leadership computing facility, the ALCF is continually breaking new ground with the development and deployment of leading-edge HPC systems and capabilities.

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

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

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

Researchers gather at an ALCF workshop to advance their application and software development efforts for Aurora.

Community Activities

Computing Conferences and Events

ALCF researchers regularly contribute to some of the world's leading computing conferences and events to share their latest advances in areas ranging from computational science and AI to HPC software and exascale technologies. In 2021, Argonne staff participated in a wide range of events including SC21; ISC High Performance; Grace Hopper Celebration; SIAM Conference on Computational Science and Engineering; Richard Tapia Celebration of Diversity in Computing Conference; IEEE International Parallel & Distributed Processing Symposium; International Conference on Parallel Processing; International Symposium on Cluster, Cloud and Grid Computing; International Workshop on OpenCL and SYCL; HPC User Forum; Lustre User Group Conference; Intel eXtreme Performance Users Group Conference; the DOE-NIH Brain Connectivity Workshop Series; and more.

COVID-19 Research Collaborations

Early in the COVID-19 pandemic, Argonne joined the national effort to mitigate this global health problem, leveraging its world-class user facilities and multidisciplinary expertise to advance our understanding of SARS-CoV-2, the virus that causes COVID-19. With funding from Congress, all 17 DOE national laboratories formed a consortium—the National Virtual Biotechnology Laboratory—that is leveraging DOE's user facilities, including the ALCF, to address key challenges in responding to the COVID-19 threat. The ALCF also joined the COVID-19 High Performance Computing Consortium, a unique private-public effort established by the White House Office of Science and Technology Policy, DOE, and IBM, that brought together government, industry, and academic leaders to provide access to world-class supercomputing resources in support of COVID-19 research. With more than 40 member institutions, the consortium aggregated a powerful pool of computing capabilities that has enabled researchers to carry out over 100 COVID-19 research projects.

Exascale Computing Project

DOE's Exascale Computing Project (ECP) is a multi-lab initiative aimed at accelerating the delivery of a capable exascale computing ecosystem. Launched in 2016, the ECP's mission is to pave the way for the deployment of the nation's first exascale systems by building an ecosystem that encompasses applications, system software, hardware technologies, architectures, and workforce development. Researchers from the ALCF and across Argonne—one of the six ECP core labs—are helping the project deliver on its ambitious goals. The laboratory has a strong presence on the ECP leadership team and has several researchers engaged in ECP projects and working groups focused on application development, software development, and hardware technology. In the workforce development space, the ECP continues to fund the annual Argonne Training Program on Extreme-Scale Computing (ATPESC), which is organized and managed by ALCF staff.

As part of the Intel Innovation Showcase at SC21, ALCF Director of Science Katherine Riley (right) joins Intel's Joe Curley to discuss extreme-scale computing.

HPC Standards and Community Groups

ALCF staff members remain actively involved in a number of HPC standards and community groups that help drive improvements in the usability and efficiency of scientific computing tools, technologies, and applications. Staff activities include contributions to the C++ Standards Committee, Cray User Group, HPC User Forum, Intel eXtreme Performance Users Group, Khronos OpenCL and SYCL Working Groups, MLPerf (HPC and Science Working Groups), MPI Forum, NITRD Middleware and Grid Infrastructure Team, oneAPI Technical Advisory Board (DPC++ and oneMKL), OpenMP Architecture Review Board, OpenMP Language Committee, Open Scalable File Systems (OpenSFS) Board, and SPEC High-Performance Group.

Performance Portability

The ALCF continued its collaboration with NERSC and OLCF to operate and maintain a website dedicated to enabling performance portability across the DOE Office of Science HPC facilities (performanceportability.org). The website serves a documentation hub and guide for applications teams targeting systems at multiple computing facilities. Staff from the DOE computing facilities also collaborate on various projects and training events to maximize the portability of scientific applications on diverse supercomputer architectures.

Vendor Collaborations

The ALCF works closely with many companies in the HPC and AI industries to develop and deploy cutting-edge hardware and software for the research community. This includes collaborating with Intel and HPE to deliver the Aurora exascale system, working with HPE to deploy the Polaris system, and partnering with NVIDIA on system enhancements and training related to ThetaGPU. Such partnerships are critical to ensuring the facility's supercomputing resources meet the requirements of the scientific computing community. In addition, the ALCF is working with several AI start-up companies, including Cerebras, Graphcore, SambaNova, Groq, and Habana, to deploy a diverse set of AI accelerators as part of the ALCF AI Testbed. The testbed, which will open up to the broader research community in 2022, is playing a key role in determining how AI accelerators can be applied to scientific research, while also allowing vendors to prepare their software and hardware for scientific AI workloads.

Engaging Current and Future HPC Users

The ALCF provides HPC training opportunities for scientists and developers, while also participating in outreach activities to inspire a new generation of computing researchers.

The convergence of artificial intelligence (AI) and data science with traditional modeling and simulation is changing the way researchers use supercomputers for scientific discovery.

To help scientists find their footing in this ever-evolving landscape, the ALCF has placed a premium on training researchers to efficiently use the latest simulation, data analysis, AI, and machine learning tools and techniques on its supercomputing resources.

In 2021, the ALCF hosted a number of training events, including virtual workshops aimed at improving application performance, interactive webinars that connect attendees with the developers of HPC systems and software, and hackathons designed to help researchers prepare their codes for exascale.

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

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

The ALCF's annual workshops connect researchers with staff and industry experts to help them improve computational performance on the facility's computing systems.

Training Users

ALCF Computational Performance Workshop

Held virtually in May, the annual ALCF Computational Performance Workshop is designed to help attendees boost application performance on ALCF systems. With dedicated access to ALCF computing resources, the three-day workshop allowed workshop participants to work directly with ALCF and invited experts to test, debug, and optimize their applications. One of the workshop's primary goals is to help researchers demonstrate code scalability for INCITE, ALCC, and ADSP project proposals, which are required to convey both scientific merit and computational readiness.

ALCF-NVIDIA GPU Hackathon

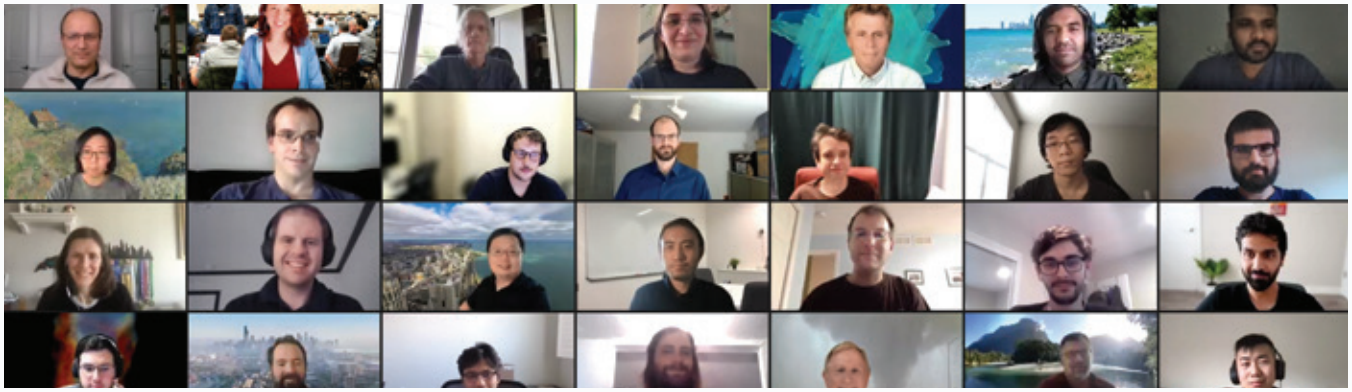
In April, the ALCF partnered with NVIDIA to host its first-ever GPU Hackathon, a virtual event designed to help developers accelerate their codes on ThetaGPU, which consists of 24 NVIDIA DGX A100 nodes, using a portable programming model, such as OpenMP, or an AI framework of their choice. Mentors were assigned to each team for the duration of the event to provide guidance on porting and optimizing their code for NVIDIA GPUs. With 15 teams participating, the event was one of NVIDIA's largest virtual GPU Hackathons to date.

ATPESC 2021

The annual Argonne Training Program on Extreme-Scale Computing (ATPESC) was held virtually for the second time in 2021. The two-week training event offers training on key skills, approaches, and tools needed to design, implement, and execute computational science and engineering applications on high-end computing systems, including upcoming exascale supercomputers. Organized by ALCF staff and funded by the ECP, ATPESC has a core curriculum that covers computer architectures; programming methodologies; data-intensive computing and I/O; numerical algorithms and mathematical software; performance and debugging tools; software productivity; data analysis and visualization; and machine learning and data science. More than 70 graduate students, postdocs, and career professionals in computational science and engineering attended this year's program. ATPESC has now hosted more than 600 participants since it began in 2013. To further extend the program's reach, ATPESC lecture videos are made publicly available on YouTube each year.

Aurora Hackathons

The Argonne-Intel Center of Excellence (COE) continued to host hands-on training events to help Aurora Early Science Program (ESP) teams develop, port, and profile their applications for the ALCF's upcoming exascale system. Events included a dungeon session involving multiple ESP projects and six hackathons. The multi-day, hands-on sessions pair ESP teams with experts from the ALCF and Intel to advance code development efforts using the Aurora software development kit, early hardware, and other exascale programming tools.



At the 2021 ALCF-NVIDIA GPU Hackathon, 15 teams worked with mentors to port and optimize their applications on ThetaGPU.

Aurora Workshop

This invitation-only workshop focused on helping ESP and ECP researchers prepare applications and software technologies for Aurora. The two-part workshop was geared toward developers and emphasized using the Intel software development kit to get applications running on testbed hardware. Teams were also given the opportunity to consult with ALCF staff and provide feedback. The workshop kicked off in October with the initial sessions focused on presentations and status updates on Aurora's hardware and software. Part two was held over two days in December and provided significant hands-on time with Aurora's testbed technologies. ALCF staff also held dedicated office hours on a range of topics from programming models to profiling tools.

Best Practices for HPC Software Developers

In 2021, the ALCF, OLCF, NERSC, and ECP continued their collaboration with the Interoperable Design of Extreme-Scale Application Software (IDEAS) project to deliver a series of webinars—Best Practices for HPC Software Developers—to help users of HPC systems carry out their software development more productively. Webinar topics included the RAJA portability suite, good practices for research software documentation, mining developmental data to improve HPC software engineering, and scientific software ecosystems and communities.

Monthly ALCF Webinars

The ALCF continued to host monthly webinars consisting of two tracks: ALCF Developer Sessions and Aurora Early Adopters Series. ALCF Developer Sessions are aimed at training researchers and increasing the dialogue between HPC users and the developers of leadership-class systems and software. Speakers in the series included developers from NVIDIA and Argonne, covering topics such as high-performance data science, kernel performance analysis, and running ThetaGPU with SDK. The Aurora Early Adopter Series is designed to introduce researchers to programming models, exascale technologies, and other tools available for testing and development work. Topics included OpenACC to OpenMP migration tool, improvements to the SYCL programming model, and writing performant parallel code with oneDPL. Both webinar series are open to the public and videos of all talks are posted to the ALCF website and YouTube channel.

Simulation, Data, and Learning Workshop

In October, the ALCF hosted its annual Simulation, Data, and Learning (SDL) Workshop, a multi-day virtual event designed to help researchers improve the performance and productivity of simulation, data science, and machine learning applications on ALCF systems. Participants had the opportunity to learn about leading-edge AI methods and technologies while working directly with ALCF staff scientists during dedicated hands-on sessions. Over the course of the workshop, attendees learned how to use deep learning tools, such as the Horovod framework, DeepSpeed library, and the Argonne-developed DeepHyper package, on ALCF computing resources.

Inspiring Students

Afro-Academic, Cultural, Technological and Scientific Olympics

In 2021, Argonne staff members served as mentors to 22 high school students participating in DuPage County's Afro-Academic, Cultural, Technological & Scientific Olympics (ACT-SO). The high school enrichment program provides an opportunity for African American students to gain real-world research experiences and explore potential careers in STEM. Five of the Argonne-mentored students went on the compete at the national ACT-SO event.

ALCF AI for Science Training Series

In 2021, the ALCF launched a new multi-week training program aimed at undergraduate and graduate students interested in taking their AI skills to a new level. The ALCF AI for Science Training Series, which kicked off in October, covers the fundamentals of using world-class supercomputers to advance the use of AI for research. Leveraging Argonne's AI expertise and ALCF supercomputing resources, the hands-on series provides a unique learning experience designed to give participants a leg up in the burgeoning field of AI for Science. Sessions cover all aspects of using supercomputers for AI, from employing Jupyter Notebooks to building data pipelines for deep learning.

ALCF Student Summer Program

Every summer, the ALCF opens its doors to a new class of student researchers who work alongside staff mentors to tackle research projects that address issues at the forefront of scientific computing. Just like last year, the internship program was virtual. The facility hosted 33 students ranging from high school seniors to Ph.D. candidates. From developing infrastructure for data and AI models to allowing researchers to easily create and interactively analyze large-scale simulations using Jupyter Notebooks, the interns had the opportunity to gain hands-on experience with some of the most advanced computing technologies in the world.

Argonne-NIU AI Camp

In July, a group of learning science experts and computer scientists from the U.S. Department of Energy's (DOE) Argonne National Laboratory and Northern Illinois University (NIU) hosted Science and Inquiry: Exploring Artificial Intelligence, a virtual AI-focused summer camp attended by regional high school students recruited through NIU's Upward Bound program. Over the course of four weeks, the camp students got a foundational introduction to AI and machine learning, including the opportunity to analyze real datasets using real analysis tools.

Big Data Camp

Argonne hosted a group of local high school juniors and seniors for its annual Big Data Camp in July. The week-long virtual event, organized by Argonne's Educational Programs Office and led by Argonne computer scientists, taught the students techniques for probing and analyzing massive scientific datasets, including data visualization methods. The attendees worked with data from the Array of Things (AoT) project and its follow-on Software-Defined Sensor Network (SAGE) project, an Argonne–University of Chicago urban sensor project, to gain hands-on experience with data-driven research.

ALCF's Joe Insley hosts students for a tour of the ALCF Visualization Laboratory.

CodeGirls@Argonne Camp

The annual CodeGirls@Argonne Camp hosts sixth- and seventh-grade girls each summer for a virtual three-day event dedicated to teaching them the fundamentals of coding. Taught by Argonne computing researchers and staff from the lab's Learning Center, the virtual camp gave students an opportunity to try out creative and computational thinking through activities that included programming robots. The camp also allowed participants to meet women scientists, who use code to solve problems, and take part in a virtual tour the ALCF's machine room and visualization lab.

Coding for Science Camp

In July, Argonne hosted its Coding for Science Camp for 30 high school freshmen and sophomores who were new to coding. The week-long camp, a joint initiative of Argonne's Educational Programs Office and the ALCF, promotes problem solving and teamwork skills through hands-on coding activities, such as coding with Python and programming a robot, and interactions with Argonne staff members working in HPC and visualization.

Hour of Code

As part of the national Computer Science Education Week (CSEdWeek) in December, ALCF staff members provide virtual talks and demos to Chicago area schools to spark interest in computer science. Working with students in classes from elementary to high school, the volunteers led a variety of activities designed to teach the basics of coding. CSEdWeek was established by Congress in 2009 to raise awareness about the need to elevate computer science education at all levels.

Introduce a Girl to Engineering Day

ALCF staff members regularly serve as mentors and volunteers for Argonne's Introduce a Girl to Engineering Day (IGED) program. The annual event, which was held virtually in 2021, gives eighth-grade students a unique opportunity to explore engineering careers via mentoring, presentations by women engineers, tours of Argonne facilities, and hands-on engineering experiments.

SC21 Student Cluster Competition

Held annually as part of the SC Conference series, the Student Cluster Competition aims to inspire undergraduate and high school students from around the world to pursue careers in HPC, demonstrating the breadth of skills, technologies, and science that it takes to build, maintain, and utilize supercomputers. Student teams are challenged to design and deploy a computing cluster, run benchmarks, and use HPC resources to meet the demands of real scientific computing applications. At SC21, ALCF staff members served on the competition committee and contributed as application experts to support and advise the student teams.

Science Careers in Search of Women

ALCF staff members continue to contribute to Argonne's annual Science Careers in Search of Women (SCSW) conference. Held virtually in 2021, the event hosts women high school students for a day of inspiring lectures, facility tours, career booth exhibits, and mentoring. SCSW provides participants with the unique experience to explore their desired profession or area of interest through interaction with Argonne's women scientists and engineers.

EXPERTISE AND RESOURCES

The ALCF's unique combination of supercomputing resources and expertise enables researchers to accelerate the pace of scientific discovery and innovation.

Ben Allen, ALCF HPC systems administration specialist, installs components in the facility's ThetaGPU machine.

ALCF Staff and Systems

The ALCF's exceptional staff and powerful supercomputing resources make the facility one of the world's premier centers for scientific computing.

The ALCF's Theta/ThetaGPU system is the engine that drove scientific advances for facility users in 2021. Recently augmented with GPUs, the supercomputer supports complex and diverse workloads involving simulation, data analytics, and artificial intelligence methods.

The arrival and installation of Polaris will soon provide a new resource for the ALCF user community. Slated to go into production in 2022, the system will give scientists and application developers a platform to test and optimize applications and software for Aurora, while also supporting some INCITE campaigns.

Cooley, the facility's visualization and analysis cluster, enables users to transform data into high-resolution images, videos, and animations, helping users to better analyze and understand the results from simulations and experiments.

The ALCF provides high-performance data storage and networking capabilities to help users manage, store, and transfer large-scale datasets generated on the facility's computing resources.

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

Expertise and Support

The ALCF has assembled a world-class team of HPC system and network administrators, computational scientists, computer scientists, data scientists, performance engineers, visualization experts, software developers, and support staff, to ensure facility users are able to get the most out of its supercomputers.

Theta is the ALCF's Intel-Cray XC40 supercomputer.

Supercomputing Resources

ALCF supercomputing resources support large-scale, computationally intensive projects aimed at solving some of the world's most complex and challenging scientific problems.

SYSTEM NAME	POLARIS	THETA: KNL NODES	THETA: GPU NODES	COOLEY
Purpose	Science Runs	Science Runs	Science Runs	Data Analysis and Visualization
Architecture	HPE Apollo 6500 Gen10+	Intel-Cray XC40	NVIDIA DGX A100	Intel Haswell
Peak Performance	44 PF (double precision)	11.7 PF	3.9 PF	293 TF
Processors per Node	3rd Gen AMD EPYC	64-core, 1.3-GHz Intel Xeon Phi 7230	2 AMD EPYC 7742	2 6-core, 2.4-GHz Intel E5–2620
GPU per Node	4 NVIDIA A100 Tensor Core	—	8 NVIDIA A100 Tensor Core	NVIDIA Tesla K80
Nodes	560	4,392	24	126
Cores	560	281,088	576	1,512
Memory	280 TB (DDR4); 87.5 TB (HBM)	843 TB (DDR4); 70 TB (HBM)	26 TB (DDR4); 8.32 TB (GPU)	47 TB (DDR4); 3 TB (GDDR5)
Interconnect	HPE Slingshot 11 with Dragonfly configuration	Aries network with Dragonfly configuration	NVIDIA QM8700 InfiniBand	FDR InfiniBand
Racks	40	24	7	6

ALCF AI-TESTBED

The ALCF AI-Testbed provides an infrastructure of next-generation AI-accelerator machines that allows researchers to evaluate the usability and performance of machine learning-based applications running on the systems. AI testbeds include:

Groq

- Tensor Streaming Processor
- >26 billion transistors, 14 nm
- Chip-to-Chip interconnect
- GroqWare software stack, Onnx

SambaNova DataScale

- Reconfigurable Dataflow Unit
- >40 billion transistors, 7 nm
- RDU-Connect
- SambaFlow software stack, PyTorch

Habana Gaudi

- Tensor processing cores
- 7nm
- Integrated 100 GbE-based interconnect
- Synapse AI Software, PyTorch, Tensorflow

Graphcore MK1

- Intelligent Processing Unit (IPU)
- 1216 IPU tiles, 14 nm
- >23 billion transistors
- IPU-Links interconnect
- Poplar software stack, PyTorch, Tensorflow

Cerebras CS-2

- Wafer-Scale Engine
- >800,000 processing cores
- 2.6 trillion transistors, 7 nm
- SwarmX fabric
- Tensorflow, PyTorch

DATA STORAGE SYSTEMS

ALCF disk storage systems provide intermediate-term storage for users to access, analyze, and share computational and experimental data. Tape storage is used to archive data from completed projects.

SYSTEM NAME	EAGLE	GRAND	THETA-FS0	THETA-FS1	SWIFT	TAPE STORAGE
File System	Lustre	Lustre	Lustre	GPFS	Lustre	—
Storage System	HPE ClusterStor E1000	HPE ClusterStor E1000	HPE Sonexion L300	IBM Elastic Storage System (ESS)	All Flash Storage Array	LTO6 and LTO8 Tape Technology
Usable Capacity	100 PB	100 PB	9 PB	7.9 PB	123 TB	300 PB
Sustained Data Transfer Rate	650 GB/s	650 GB/s	240 GB/s	400 GB/s	48 GB/s	—
Disk Drives	8,480	8,480	2,300	7,260	—	—

NETWORKING

Networking is the fabric that ties all of the ALCF's computing systems together. InfiniBand enables communication between system I/O nodes and the ALCF's various storage systems. The Production HPC SAN is built upon NVIDIA Mellanox High Data Rate (HDR) InfiniBand hardware. Two 800-port core switches provide the backbone links between 80 edge switches, yielding 1600 total available host ports, each at 200 Gbps, in a non-blocking fat-tree topology. The full bisection bandwidth of this fabric is 320 Tbps. The HPC SAN is maintained by the NVIDIA Mellanox Unified Fabric Manager (UFM), providing Adaptive Routing to avoid congestion, as well as the NVIDIA Mellanox Self-Healing Interconnect Enhancement for InteLligent Datacenters (SHIELD) resiliency system for link fault detection and recovery.

When external communications are required, Ethernet is the interconnect of choice. Remote user access, systems maintenance and management, as well as high performance data transfers are all enabled by the Local Area Network (LAN) and Wide Area Network (WAN) Ethernet infrastructure. This connectivity is built upon a combination of Extreme Networks SLX and MLXe routers and NVIDIA Mellanox Ethernet switches.

ALCF systems connect to other research institutions over multiple 100 Gbps Ethernet circuits that link to many high performance research networks, including local and regional networks like the Metropolitan Research and Education Network (MREN), as well as national and international networks like the Energy Sciences Network (ESnet) and Internet2.

JOINT LABORATORY FOR SYSTEM EVALUATION

Through Argonne's Joint Laboratory for System Evaluation (JLSE), the ALCF provides access to leading-edge testbeds for exploratory research aimed at evaluating future extreme-scale computing systems, technologies, and capabilities. JLSE testbeds include:

Arcticus, DevEP, Iris: Intel discrete and integrated GPU testbeds for ECP and ESP projects to develop, optimize, and scale applications and software for Aurora

Aurora Software Development Kit: Frequently updated version of the publicly available Intel oneAPI toolkit for Aurora development

Arm Ecosystem: Apollo 80 Fujitsu A64FX Arm system, NVIDIA Ampere Arm and A100 test kits, and an HPE Comanche with Marvell ARM64 CPU platform provide an ecosystem for porting applications and measuring performance on next-generation systems

Atos Quantum Learning Machine: Platform for testing and developing quantum algorithms and applications

Intel Xeon Clusters: Cascade Lake, Skylake, and Cooper Lake Xeon clusters enable a variety of research activities, including testing AI and learning applications

NVIDIA and AMD GPUs: Clusters of NVIDIA V100, A100, and A40 GPUs, and AMD MI50 and MI100 GPUs for preparing applications for heterogeneous computing architectures

Presque: Intel DAOS nodes for testing the Aurora storage system

ALCF Team

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

Science

Computational scientists with multidisciplinary domain expertise work directly with ALCF users to maximize and accelerate their research efforts. In addition, the ALCF team applies broad expertise in data science, machine learning, data visualization and analysis, and mathematics to help application teams leverage ALCF resources to pursue data-driven discoveries.

With a deep knowledge of the ALCF computing environment and experience with a wide range of numerical methods, programming models, and computational approaches, staff scientists and performance engineers help researchers optimize the performance and productivity of simulation, data, and learning applications on ALCF systems.

Operations

The ALCF's HPC systems administrators manage and support all ALCF computing systems, ensuring users have stable, secure, and highly available resources to pursue their scientific goals. This includes the ALCF's production supercomputers, supporting system environments, storage systems, and network infrastructure. The team's software developers create tools to support the ALCF computing environment, including software for user account and project management, job failure analysis, and job scheduling.

User support specialists provide technical assitance to ALCF users and manage the workflows for user accounts and projects. In the business intelligence space, staff data architects assimilate and verify ALCF data to ensure accurate reporting of facility information.

Technology

The ALCF team plays a key role in designing and validating the facility's next-generation supercomputers. By collaborating with compute vendors and the performance tools community, staff members ensure the requisite programming models, tools, debuggers, and libraries are available on ALCF platforms. The team also helps manage Argonne's Joint Laboratory for System Evaluation, which houses next-generation testbeds that enable researchers to explore and prepare for emerging computing technologies.

ALCF computer scientists, performance engineers, and software engineers develop and optimize new tools and capabilities to facilitate science on the facility's current and future computing resources. This includes the deployment of scalable machine learning frameworks, in-situ visualization and analysis capabilities, data management services, workflow packages, and container technologies. In addition, the ALCF team is actively involved in programming language standardization efforts and contributes to cross-platform libraries to further enable the portability of HPC applications.

Outreach

ALCF staff members organize and participate in training events that prepare researchers for efficient use of leadership computing systems. They also participate in a wide variety of educational activities aimed at cultivating a diverse and skilled HPC community for the future. In addition, staff outreach efforts include facilitating partnerships with industry and communicating to external audiences the impactful research enabled by ALCF resources.

Staff News

Marta García Martínez was recognized with the 2021 UChicago Argonne Board of Governors Pinnacle of Education Award.

Adams receives DOE Early Career Research Program Award

Corey Adams, an ALCF computer scientist with a joint appointment in Argonne's Physics division, received a DOE Early Career Research Program Award, for his research on the construction of a background-free, normal-ordering neutrino-less double beta decay demonstrator. Adams was one of 83 scientists nationwide to receive the prestigious award, which provides each recipient with at least $500,000 per year for five years to advance their research. Now in its 12th year, the program is designed to bolster the nation's science workforce by providing financial support to exceptional researchers during their critical early-career years.

Brown named Argonne's first Walter Massey Fellow

Kevin Brown, ALCF postdoctoral researcher, was awarded Argonne's first Walter Massey Fellowship. The new fellowship recognizes an exceptional scientist committed to diversity, equity and inclusion, who is at the early stage of their research career. As the Walter Massey Fellow, Brown will continue his research in network performance analysis and simulation as the PI of a three-year project titled "Improving Data Movement Performance for Emerging AI and Climate Science Workloads on Future Supercomputers."

García Martínez receives Pinnacle of Education Award

Marta García Martínez, Argonne computational scientist, was recognized with the 2021 UChicago Argonne Board of Governors Pinnacle of Education Award for her exceptional contributions and continuous efforts to science education and outreach. In addition to her role as an ALCF catalyst, García Martínez has served as program director of the Argonne Training Program on Extreme-Scale Computing; program chair of the Exascale Computing Project Annual Meeting; an organizer and contributor to multiple HPC training events including ALCF user workshops and the nation-wide Petascale Computing Institute; and a volunteer, speaker, and mentor for student outreach events, such as Introduce a Girl to Engineering Day, Science Careers in Search of Women, Hour of Code, and the Illinois Middle School Regional Science Bowl.

ALCF and IIT research team receive Best Paper Award at CCGrid2021

ALCF's Huihou Zheng and Venkat Vishwanath teamed up with Illinois Institute of Technology researchers Hariharan Devarajan, Anthony Kougkas, and Xian-He Sun for a study that was awarded best paper at the Institute of Electrical and Electronics Engineers (IEEE)/ Association for Computing Machinery (ACM) International Symposium on Cluster, Cloud and Internet Computing (CCGrid). The team's paper, "DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications," presented a new benchmark to investigate the data I/O patterns of various deep learning applications running on supercomputers.

ALCF researchers' paper selected as Editor's Pick

Argonne's Romit Maulik, Bethany Lusch, and Prasanna Balaprakash published a paper, "Reduced-order modeling of advection-dominated systems with recurrent neural networks and convolutional autoencoders" in Physics of Fluids that was selected as an Editor's Pick.

ALCF team recognized with DOE Secretary of Energy's Achievement Award

ALCF Director Michael Papka, ALCF Director of Science Katherine Riley, and the lab's High-Performance Computing Resource Team were recognized with a DOE Secretary of Energy's Achievement Award for their work in mobilizing supercomputing resources to accelerate research into treatments and strategies to combat the COVID-19 pandemic.

Staff Spotlights

KYLE SCHMITT
HPC Systems Administrator

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

With a shared passion for research and innovation, ALCF staff members are helping to shape the future of supercomputing. The following pages highlight six staff members and some of their notable contributions in 2021.

Kyle Schmitt joined ALCF in 2020 as a Systems Integration Administrator for the Joint Laboratory for Systems Evaluation (JLSE). The JLSE manages resources for Argonne’s research community to support the evaluation of future hardware and software platforms. In his role, Kyle works to maintain a range of experimental hardware and software environments for research; improve science productivity on current and future Argonne Leadership Computing Facility (ALCF) platforms; investigate alternative approaches to current and future deployments within ALCF; and help to drive standards in forums on benchmarking, programming models, programming languages, and memory technology.

Kyle manages a diverse set of machines within the JLSE, featuring various accelerators for users to test under specific hardware combinations and environments. Example systems include a platform with 64bit ARM CPUs with Nvidia-A100 GPUs, or nodes that use the same Fujitsu ARM platform as Japan’s Fugaku supercomputer. Kyle architects, installs, and maintains the systems within the JLSE, making him a frequent visitor to the Building 240 datacenter.

In 2021, Kyle was part of a project to design and host a number of testbeds for Aurora, ALCF’s upcoming exascale computer. One such system is called Arcticus, a precursor to the Aurora. Another is called Presque, a DAOS testbed, which is the same system as a newly developed fast IO system for Aurora.

COREY ADAMS
Computer Scientist

VICTOR MATEEVITSI
Assistant Computer Scientist

Corey Adams joined the ALCF in 2016 as an Assistant Computer Scientist with a joint appointment in the Argonne Physics Division. Since joining the lab, Corey's work has primarily focused on the intersection of deep learning, HPC, and fundamental physics.

Currently, Corey works on scaling algorithms for fundamental physics research with machine learning, including segmentation of high-resolution particle physics datasets, sparse convolutional networks for 3D datasets, and surrogate models for nuclear theory calculations. He is also head of the postdoc committee, where he oversees the hiring of postdocs and posting of new positions, and interviews new postdoc candidates.

Corey continues to lead efforts to deploy advanced deep learning frameworks on Aurora, the forthcoming exascale system set for delivery next year at the ALCF. His research encompassed contributions to Aurora non-recurring engineering (NRE) efforts that target Aurora Early Science Program (ESP) projects, including connectomics brain-mapping work and the CANDLE virtual drug response prediction and cancer treatment application, in addition to applications for astrophysics, neutrino physics, lattice quantum chromodynamics, Argonne's Advanced Photon Source (APS), and the Large Hadron Collider.

He also co-organized the 2021 Computational Performance Workshop, an virtual experience designed to help researchers boost application performance and achieve computational readiness on ALCF systems by working with ALCF and industry professionals through collaborative online sessions.

In 2021, Corey received a DOE award for his research on the construction of a background-free, normal-ordering neutrino-less double beta decay demonstrator. Adams' research was selected for funding by DOE's Office of Nuclear Physics.

Victor Mateevitsi joined Argonne in 2020 as a Computer Scientist with ALCF's Visualization Team, where he helps domain scientists gain insights into data and uncover key discoveries through the power of visualization. Victor's work is a combination of left and right brain activities: sometimes he writes software that runs on leadership-scale machines, others he visualizes complex multivariate data. He is currently involved with the Exascale Computing Project (ECP) initiative, where he prepares science codes for in situ capabilities for ALCF's upcoming exascale supercomputer, Aurora. Furthermore, he works with scientists from CPS to instrument computational fluid dynamics codes with SENSEI—an in-situ and in-transit visualization library—and to perform large-scale science runs. In between projects, you can find him in the Metaverse, exploring Augmented Reality as a science analysis tool.

Committed to his education and outreach efforts, Victor has been a member of the Argonne Action Collaborative that creates a safe space to address and prevent gender and sexual harassment. He is also an instructor at the Big Data Camp, and a mentor at the Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) High School Research Program—with one of his students having won Gold in the DuPage competition and Silver at Nationals in 2021. Finally, Victor is the founding member and chair of the local Chicago ACM SIGCHI chapter, and served as a co-chair for the 2021 IEEE VIS Conference's Satellite Event held in Chicago. When he's not online, he's on skates, playing ice hockey indoors and outdoors around Chicago.

SAUMIL PATEL
Assistant Computational Scientist

MURALI EMANI
Assistant Computer Scientist

Saumil Patel joined the ALCF in 2016 as a multi-divisional postdoctoral appointee. During this time, he worked with scientists in the Mathematics and Computer Science (MCS) and Energy Systems (ES) divisions to develop numerical algorithms and workflows in the open-source, computational fluid dynamics (CFD) solver, Nek5000, for investigating turbulence inside internal combustion engines. In 2021, Saumil served as a co-PI of an INCITE project that generated highly resolved data to improve our understanding of cycle-to-cycle phenomena in engines. This research is currently being leveraged to develop improved heat transfer models that can be used by original equipment manufacturers to design more efficient engines.

Saumil's day-to-day activities include acting as a catalyst for INCITE projects. He works with the project PIs to ensure they can compile code and run their simulations on Theta. Saumil also works with science teams to enable their codes to run at scale on ALCF resources. In addition, he supervises Umesh Unnikrishnan, an ALCF postdoctoral appointee working to optimize the libParanumal library for hypersonic applications on the upcoming Aurora machine.

Saumil also works on multiple initiatives within the Exascale Computing Project (ECP). In 2021, he worked with ALCF's Kris Rowe, a performance engineer, and Intel technical staff to develop benchmarks that contributed to the development of the OCCA library for running scientific software on Intel GPUs. He has also collaborated with Silvio Rizzi, a member of ALCF's visualization team, to enable in-situ visualization capabilities for ECP simulation codes like nekRS. In addition, Saumil is part of the Exascale ProxyApps project where he and Argonne computational scientist Ramesh Balakrishnan lead an effort to develop an open source, CFD solver based on the lattice Boltzmann method.

Murali Emani works at the intersection of machine learning and computing systems to enhance the scalability of machine learning and deep learning methodologies and frameworks on emerging supercomputers for scientific applications. His research interests include parallel programming models, HPC, scalable machine learning, runtime systems, emerging HPC architectures, and online adaptation.

Some of Murali's current projects include developing performance models to identify and address bottlenecks, as well as scaling machine learning and deep learning frameworks on emerging supercomputers for scientific applications. He also co-designs the emerging hardware architectures to scale up machine learning algorithms, works on benchmarking ML/DL frameworks and methods on HPC systems, ports machine learning applications to Aurora, and develops HPC-FAIR framework for reproducible AI models for HPC.

Murali's research projects have been published in various notable conferences such as PLDI, PACT, CGO, MLHPC. He also co-leads the AI Testbed, where he and his team explore the performance efficiency of AI accelerators for scientific machine learning applications and work closely with domain scientists and vendors. A paper he co-authored on coupling Cerebras accelerators with leadership-scale supercomputers at NERSC and ALCF was selected as a finalist for the ACM Gordon Bell Special prize for HPC-based COVID-19 research.

Murali serves as a co-chair for MLPerf HPC group at MLCommons to benchmark large scale ML on HPC systems, also serving in the program committee for conferences such as IPDPS and PACT and chaired several workshops and Birds of a Feather sessions at Supercomputing and MLSys.

LALITHA MANTRALA
User Experience Analyst

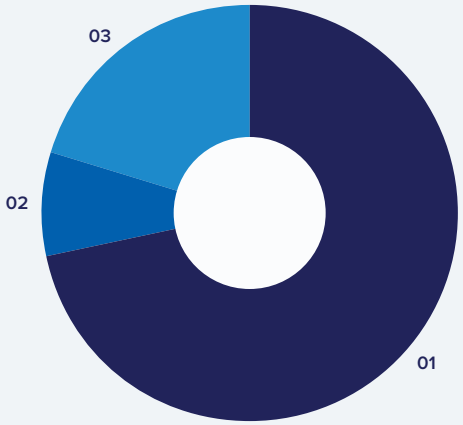
Since joining the lab in 2009, Avanthi "Lalitha" Mantrala has become a senior member of the ALCF's User Experience (UX) team. Lalitha's responsibilities include providing support to ALCF users throughout the lifecycle of their projects, facilitating rapid system access to approved users, triaging technical issues, and leading ramp-ups of various ALCF allocation programs. In this role, she contributes to improving the overall user experience of researchers using ALCF supercomputers to pursue advances in science and engineering.

Lalitha also leads various collaborative projects that require coordination among different ALCF teams. A recent example is the effort to set up a new global filesystem for ALCF users and projects. As part of that work, Lalitha led the team responsible for performing functional validation of the new community data-sharing service. Lalitha and her collaborators were recognized with an Impact Argonne Award for their extraordinary efforts.

Lalitha continues to contribute to projects critical to the future of the facility, including leading the ALCF's Operational Assessment Review (OAR) and co-leading the training and support preparations for the early science users of Aurora.

In addition to her day-to-day work, Lalitha participates in several outreach and mentoring activities across the laboratory. She enjoys working with students as a volunteer for Argonne's annual Introduce a Girl to Engineering Day and Science Careers in Search of Women programs. Lalitha is part of an Argonne diversity and inclusion committee and a steering committee member for the lab's Women in Science and Technology (WIST) group, where she worked on creating a pilot program focused on Mentoring Circles.

ALCF STAFF NUMBERS



01 Staff Members

117

02 Postdoctoral Researchers

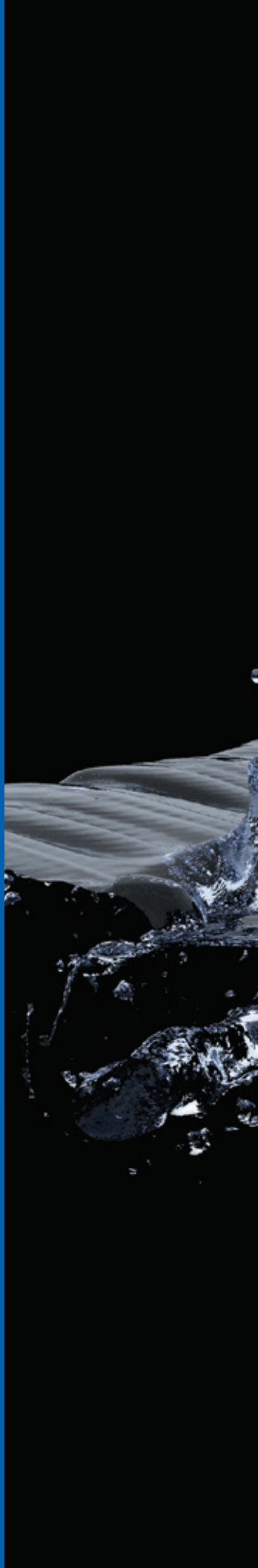
13

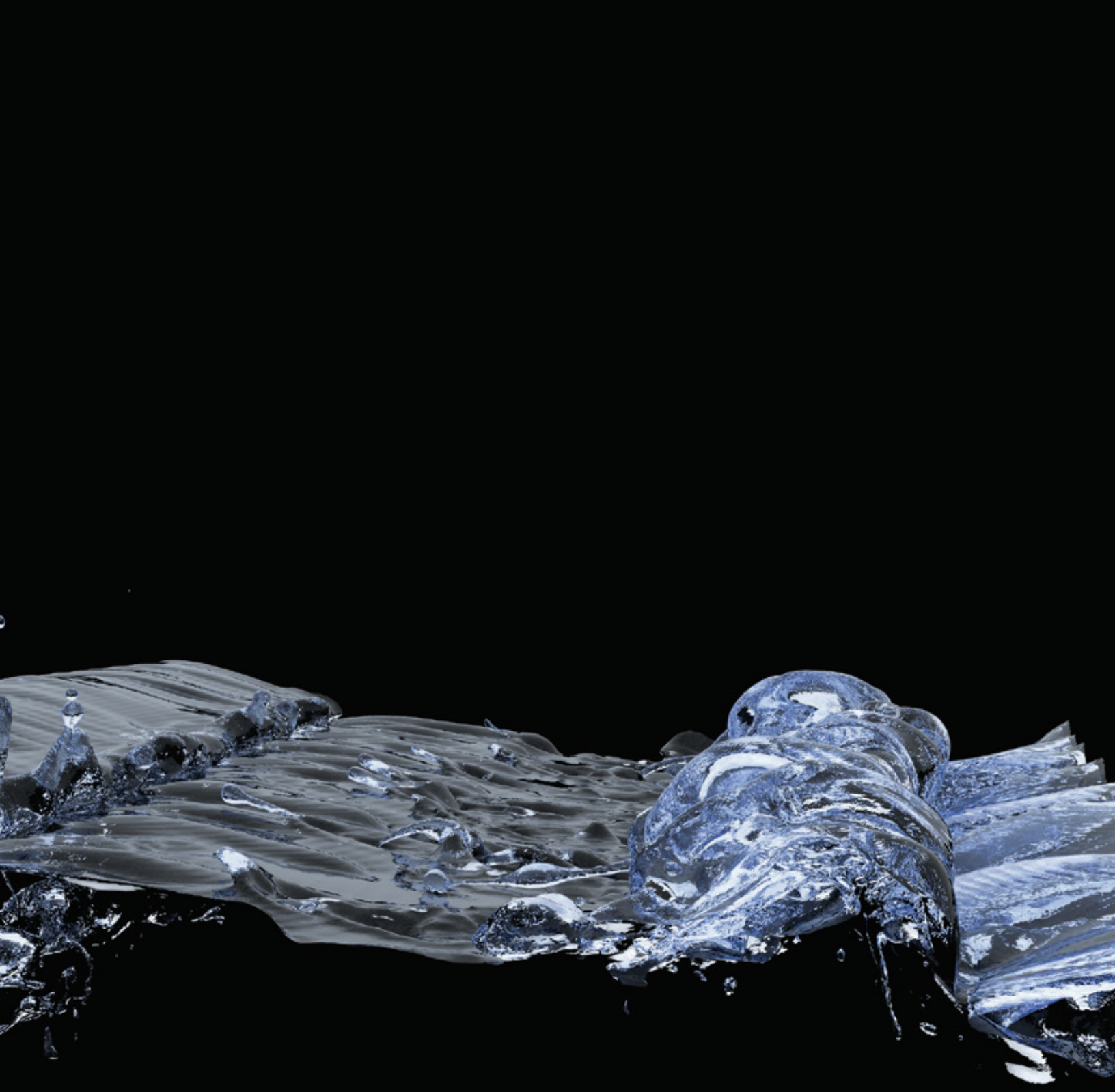
03 Summer Students

33

SCIENCE

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





Parviz Moin of Stanford University is leading an ALCC project that is using ALCF computing resources to perform high-fidelity simulations of bubble breakup and gas dissolution in turbulent oceanic environments. This image shows the generation of drops and bubbles from an oceanic breaking wave obtained from a geometric volume-of-fluid numerical simulation. The snapshot highlights the multiscale nature of wave-breaking phenomena. *Image: WH Ronald Chan, University of Colorado Boulder; Suhas S. Jain, Ali Mani, Shahab Mirjalili, Parviz Moin, and Javier Urzay, Stanford University*

Accessing ALCF Resources for Science

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

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

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

Application Programs

ADSP

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

ESP

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

Allocation Programs

INCITE

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

ALCC

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

DIRECTOR'S DISCRETIONARY

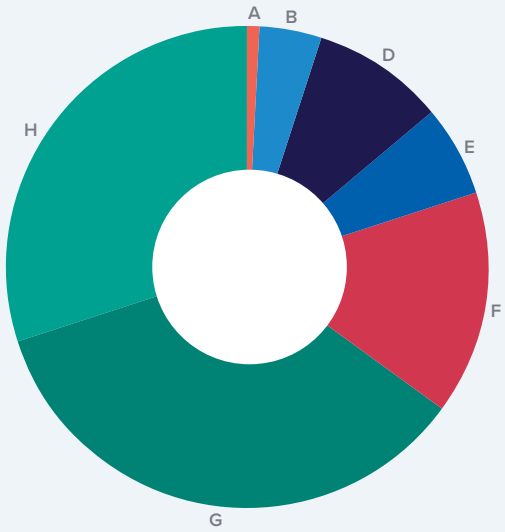
Director's Discretionary projects are dedicated to leadership computing preparation, INCITE and ALCC scaling, and application performance to maximize scientific application efficiency and productivity on leadership computing platforms.

INCITE/ALCC BY DOMAIN

2021 INCITE

17.8M NODE HOURS

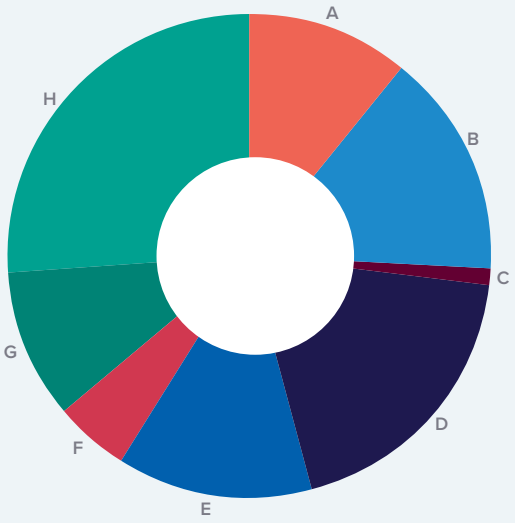
A	Biological Sciences	1 %
B	Chemistry	4
C	Computer Science	–
D	Earth Science	9
E	Energy Technologies	6
F	Engineering	15
G	Materials Science	35
H	Physics	30



2021 ALCC

7.3M NODE HOURS

A	Biological Sciences	11 %
B	Chemistry	15
C	Computer Science	1
D	Earth Science	19
E	Energy Technologies	13
F	Engineering	5
G	Materials Science	10
H	Physics	26

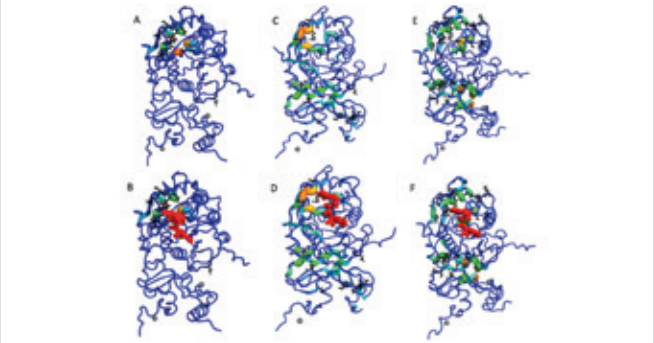


ALCC data are from calendar year 2021.

Biological Sciences | Simulation

Finding Druggable Sites in SARS-CoV-2 Proteins Using Molecular Dynamics and Machine Learning

PI Albert Lau, Johns Hopkins School of Medicine
AWARD Director's Discretionary
HOURS Theta: 250,000 Million Node-Hours



Druggable sites of SARS-CoV-2 MTase protein predicted by TACTICS workflow: open pockets (top) and ligand-bound pockets (bottom) with residues of drug binding sites and ligand emphasized in bold color. *Image: Reproduced from J. Chem. Inf. Model., 61, 2897 (2021)*

A molecular biophysics group at Johns Hopkins School of Medicine developed a joint computational and experimental approach using machine learning to accelerate novel drug discovery, especially in the treatment of the disease COVID-19 associated with the novel coronavirus SARS-CoV-2.

CHALLENGE

Coronavirus disease 2019 (COVID-19) is caused by a novel coronavirus called Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) and was declared a pandemic by the World Health Organization on March 11, 2020. To date, only a few repurposed drugs have shown limited benefits in critically ill patients. The challenge these researchers tackled was the ability to accurately and efficiently determine where the drug-binding sites are located on target proteins.

APPROACH

REST2 (Replica Exchange Solute Tempering–2nd Generation) is a powerful sampling enhancement algorithm that accelerates infrequent conformational transitions of macromolecules by augmenting interaction energy fluctuations of a simulated system. Simulations with REST2 were critical in this project for searching all important conformational transitions that require timescales beyond general simulation methodologies. Multiple copies (replicas) of each simulated protein system were generated by augmenting the interactions of the proteins to different effective temperatures. The team then applied TACTICS, a newly developed machine learning algorithm, to explore the druggability of various sites in the protein in conformations generated by REST2. Molecular dynamics trajectories were first processed by a clustering algorithm, and then important conformations were analyzed with a random forest algorithm to identify relevant protein residues in conformations likely to bind drugs. Calculations were performed using Theta.

RESULTS

TACTICS successfully identified druggable sites observed by previous experiments and refined the local residues and conformations likely to be important for binding at these sites. Moreover, TACTICS predicted several additional druggable sites.

IMPACT

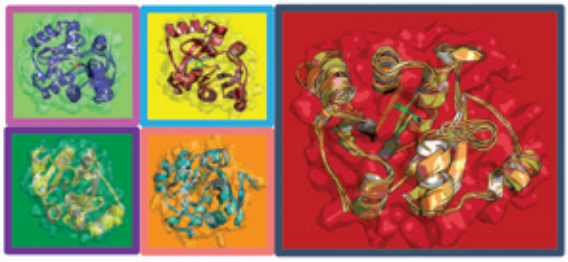
General oral medications are expected to present significant usage flexibility and lower manufacturing, transportation, and storage costs than antibodies for COVID-19 control. Development of a high-fidelity, high-resolution, all-atom simulation and modeling methodology that can predict all drug binding sites as well as their local conformations is a key step towards rational drug design. The TACTICS workflow developed here—which is capable of detecting "cryptic" binding sites that are difficult to detect without a binding ligand—opens the door for identifying potential druggable sites.

PUBLICATIONS
Evans, D. J., R. A. Yovanno, S. Rahman, D. W. Cao, M. Q. Beckett, M. H. Patel, A. F. Bandak, and A. Y. Lau. "Finding Druggable Sites in Proteins Using TACTICS," *Journal of Chemical Information and Modeling* (June 2021), ACS.

Biological Sciences | Data, Learning

Observing the SARS-CoV-2 Replication-Transcription Machinery in Action

PI Arvind Ramanathan, Argonne National Laboratory
AWARD INCITE
HOURS Theta: 81,000 Node-Hours



AI-driven MD simulations provide insights into how different ligands modulate the binding region of the viral ADP-ribose-1"-phosphatase protein. Ligands are shown in stick like representation and the protein is shown as a cartoon ensemble Note that each ligand has an effect on distinct regions of the protein. *Image: Argonne National Laboratory*

This project seeks to address the fundamental biological mechanisms, including self-replication, of the SARS-CoV-2 virus and associated COVID-19 disease, while simultaneously targeting the entire viral proteome to identify potential therapeutics.

CHALLENGE

Collaborating closely with their colleagues at Argonne's Advanced Photon Source, the researchers leverage high-performance computers to examine the intricacies of SARS-CoV-2 self-reproduction. The coronavirus uses a precisely coordinated process known as the replication-transcription complex to reproduce at high speed when it invades a host's cells. Beyond eluding simple observation, the process represents a system of some 2 million atoms, making its study a tall order.

APPROACH

Initial data for this work were obtained from cryo-electron microscopy, a technique that flash-freezes molecules and bombards them with electrons to generate 3D images. In performing their simulations, the team used a hierarchical AI framework running on the workflow engine Balsam to distribute their code across four leadership computing systems, one of which was Theta. Access to the ALCF AI Testbed enabled the team to train deep learning models that were coupled with the leadership systems. The approach built on the team's previous Gordon Bell-winning simulation of spike protein behavior in the SARS-CoV-2 virus.

RESULTS

The team's innovative workflow bridges gaps in resolution and timescale that enable it to capture important dynamics in the SARS-CoV-2 replication transcription process. The results were captured in a paper that was a finalist for the Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, as was another publication from the same team elucidating the virus's infiltration of the human immune system. The simulations performed provided information uncapturable by cryo-electron microscopes, meaningfully reconstructing viral motions that would otherwise remain incomprehensible.

IMPACT

The team's research has grown our understanding of the SARS-CoV-2 virus and the COVID-19 disease. Elucidating the virus's behavior and mechanisms can help identify effective new treatments and therapies for combatting its spread and severity, and the research potentially could lead to the design of new generative models based on reinforcement learning for both small molecules and antibodies.

PUBLICATIONS

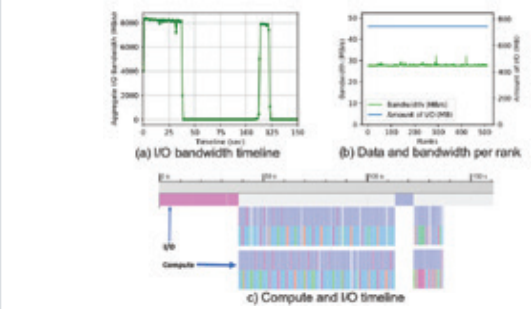
Casalino, L., A. Dommer, Z. Gaieb, E. P. Barros, T. Sztain, S.-H. Ahn, A. Trifan, A. Brace, A. Bogetti, H. Ma, H. Lee, M. Turilli, S. Khalid, L. Chong, C. Simmerling, D. J. Hardy, J. D. C. Maia, J. C Phillips, T. Kurth, A. Stern, L. Huang, J. McCalpin, M. Tatineni, T. Gibbs, J. E. Stone, S. Jha, A. Ramanathan, and R. E. Amaro. "AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics," *International Journal of High Performance Computing Applications* (April 2021), SAGE Publishing.

Trifan, A., D. Gorgun, Z. Li, A. Brace, M. Zvyagin, H. Ma, A. Clyde, D. Clark, M. Salim, D. J. Hardy, T. Burnley, L. Huang, J. McCalpin, M. Emani, H. Yoo, J. Yin, A. Tsaris, V. Subbiah, T. Raza, J. Liu, N. Trebesch, G. Wells, V. Mysore, T. Gibbs, J. Phillips, S. C. Chennubhotla, I. Foster, R. Stevens, A. Anandkumar, V. Vishwanath, J. E. Stone, E. Tajkhorshid, S. A. Harris, and A. Ramanathan. "Intelligent Resolution: Integrating Cryo-EM with AI-Driven Multi-Resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action," *International Journal of High Performance Computing Applications* (preprint), SAGE Publishing.

Computer Science | Simulation, Learning

DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications

PI Huihuo Zheng and Venkatram Vishwanath, Argonne National Laboratory
AWARD Director's Discretionary
HOURS Theta: 4,000 Node Hours



I/O behavior of CANDLE NT3 DL application: Figure a) shows the aggregate bandwidth achieved of 8 GB/s for the applications. Figure b) depicts the distribution of I/O (i.e., 700 MB) and the achieved bandwidth (28 MB/s) across ranks. Figure c) is a merged timeline that shows I/O and compute do not overlap. *Image: Argonne National Laboratory and Illinois Institute of Technology*

The emergence of deep learning techniques has provided a new tool for accelerating scientific exploration and discoveries. A group of researchers from the Argonne Leadership Computing Facility (ALCF) and the Illinois Institute of Technology (IIT) set out to improve the efficiency of deep learning-driven research by developing a new benchmark, named DLIO, to investigate the data input/output (I/O) patterns of various deep learning applications.

CHALLENGE

With the increase in the deep learning processing capabilities in current and future processors, the gap between computation and I/O for deep learning is expected to grow even further. The focus of current DL benchmarks has been primarily limited to understand the compute performance of deep learning applications, however, the end-to-end performance, including data processing and I/O, isn't well understood and lacking at scale. The researchers aim to provide a deeper dive into various scientific DL applications in HPC and build a representative benchmark which can further research and development.

APPROACH

DLIO aims to accurately characterize the behavior of scientific DL applications and guide data-centric optimizations on modern HPC systems. To develop this, the team first characterized the behavior of modern scientific DL applications currently running on production supercomputers at Argonne Leadership Computing Facility (ALCF). In order to acquire a holistic view of how data is accessed in DL applications, the team utilized both high-level and low-level I/O profiling tools, including profilers from deep learning frameworks such as TensorFlow together with I/O profilers such as Darshan, to provide a more complete picture of the end-to-end application. DLIO incorporates the observed I/O behavior of these applications and is able to emulate an application's I/O performance. The benchmark suite was validated by statistically comparing the generated I/O behaviors with the application's pattern. Additionally, DLIO provides a highly tunable data-generation toolkit that can be used to project the behavior of DL applications at scale.

RESULTS

The team found deep-learning applications use scientific data formats that are not well-supported by deep-learning frameworks; however, with their representative benchmark DLIO, this work identified optimizations that can increase I/O efficiency by a factor of six over on existing applications.

IMPACT

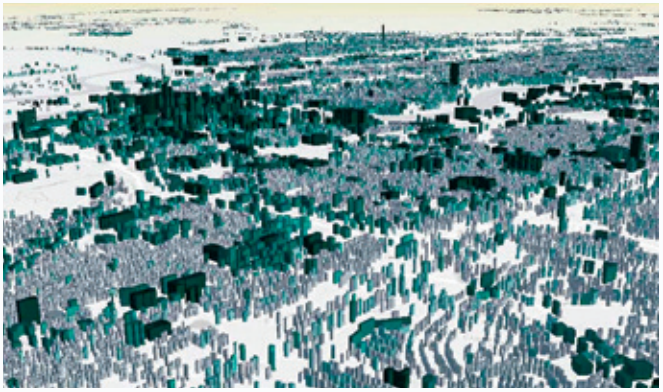
Using the DLIO benchmark, application developers can identify potential I/O bottlenecks in their applications on leadership systems and guide optimizations to boost the I/O performance and the overall time-to-solution. System architects can use this tool to aid the design of future systems and to evaluate the impact of various design choices on scientific machine learning applications.

PUBLICATIONS
Devarajan, H., H. Zheng, A. Kougkas, X.-H. Sun, and V. Vishwanath. "DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications," *2021 IEEE/ACM 21st International Symposium on Cluster, Cloud and Internet Computing (CCGrid)* (May 2021), Melbourne, Australia, IEEE.

Energy Technologies | Simulation, Learning

Automatic Building Energy Modeling

PI Joshua New, Oak Ridge National Laboratory
AWARD ALCC
HOURS Theta: 300,000 Node Hours



The Automatic Building Energy Modeling (AutoBEM) software is capable of detecting buildings, generating models, and simulating building energy use for every building in very large geographical areas. *Image: Joshua New, Oak Ridge National Laboratory*

Residential and commercial buildings consume nearly three-quarters of U.S. electricity. Simulating that energy use on a broad scale can help identify ways to reduce it, cutting greenhouse gas emissions in the process. A research team from Oak Ridge National Laboratory (ORNL) is using ALCF supercomputing resources to model individual building energy use at a national scale for the first time.

CHALLENGE

Creating an energy picture of a large network of buildings—while retaining actionable information at the individual building level—can illuminate areas of opportunity for deploying energy-saving technologies. However, many efforts to model buildings rely on representative prototypes of common residential and commercial buildings such as offices, warehouses, and schools. Gaps remain between what a computer model will predict and what real life will reflect in terms of energy use. To narrow those gaps, models need to be validated with actual energy use data.

APPROACH

The ORNL team has developed the Automatic Building Energy Modeling (AutoBEM) software, which is used to detect buildings, generate models, and simulate building energy use for very large areas. With this ALCC project, the researchers have used the ALCF's Theta supercomputer to leverage existing organizational relationships, scalable data sources, and unique algorithms to build nation-scale building energy models.

RESULTS

In a study published in *Energies*, the researchers assessed energy use across more than 178,000 buildings in Chattanooga, Tennessee. The team partnered with a municipal utility to create a digital twin of each building. The models resulting from different data sources and algorithms were compared to the utility's information on energy use for every building, down to 15-minute intervals. Then they projected eight building improvements on energy use, demand, cost, and emissions. This involved bringing all buildings up to the state's current building code and included roof insulation, lighting changes, and improvements to heating and cooling efficiency, as well as more intelligent control options via smart thermostats and water heaters.

In addition, the researchers used Theta to create a publicly available data repository that includes models of 122.9 million buildings (98 percent of the nation's building stock). To do so, their AutoBEM tool leveraged DOE's open-source EnergyPlus building simulation and OpenStudio software. The models are made available by state and county for others to modify for their own purposes.

IMPACT

This project is helping to identify effective energy-savings measures to create a more sustainable and resilient built environment. The team is working with companies to make the resulting building energy models and analysis free and publicly available, stimulating private sector activity towards more grid-aware energy efficiency alternatives.

PUBLICATIONS

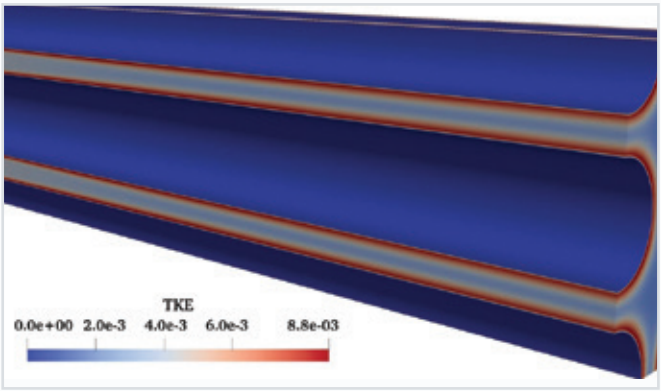
Bass, B., J. New, and W. Copeland. "Potential Energy, Demand, Emissions, and Cost Savings Distributions for Buildings in a Utility's Service Area," *Energies* (December 2020), MDPI.

New, J., M. Adams, A. Berres, B. Bass, and N. Clinton. "Model America – Data and Models of Every U.S. Building," *ORNL Constellation* (April 2021), U.S. Department of Energy.

Energy Technologies | Simulation

ExaSMR: Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors

PI Steve Hamilton, Oak Ridge National Laboratory
AWARD Aurora Early Science Program and Exascale Computing Project
HOURS Theta: 31,000 Node-Hours



Rendering of solvated DNA undergoing proton irradiation. *Image: Christopher C. Shepard, University of North Carolina at Chapel Hill*

The whirls and eddies of coolant that flow around the fuel pins play a critical role in determining the reactor thermal and hydraulics performance and give much needed information to nuclear engineers about how to best design future nuclear reactor systems, both for their normal operation and for their stress tolerance.

However, understanding the physical behavior inside an operating nuclear reactor can only be accomplished via simulation due to the high-pressure, high-temperature, and radioactive environment inside a reactor core.

Large-scale high-resolution models yield more informative simulations that can help eventually build a new, intrinsically safe nuclear reactor. To this end, computational scientists and nuclear engineers at DOE laboratories are working to complete the first ever full-core pin-resolved computational fluid dynamics (CFD) model of a small modular reactor (SMR) under the DOE's Exascale Computing Project.

CHALLENGE

The ultimate research objective of ExaSMR is to carry out the full-core multi-physics simulations that couple both CFD and neutron dynamics on the upcoming cutting-edge exascale supercomputers, such as the forthcoming Aurora system.

APPROACH

The driver application, ENRICO, performs inline coupling of the Nek5000 CFD module with Monte Carlo (MC) through a common API that supports two MC modules—Shift, which is targeting the Frontier architecture at ORNL, and OpenMC, which is targeting the Aurora system at ANL.

RESULTS

This work has resulted in the first ever full-core pin-resolved CFD simulations of SMR and application of $\kappa - \tau$ RANS model in a GPU-oriented CFD flow-solver, NekRS. As described in a *Nuclear Engineering and Design* paper detailing the team's project, it was found that the mechanisms by which the coolant mixes throughout the core remain regular and relatively consistent, enabling the researchers to leverage high-fidelity simulations of the turbulent flows in a section of the core to enhance the accuracy of the core-wide computational approach.

A key aspect of the modeling of SMR fuel assemblies is the presence of spacer grids, which an important role in pressurized water reactors by creating turbulent structure and enhancing the capacity of the flow to remove heat from the fuel rods containing uranium. Instead of creating a computational grid resolving all the local geometric details, the researchers developed a mathematical mechanism to reproduce the overall impact of these structures on the coolant flow without sacrificing accuracy. The mathematical mechanism created by the researchers enables them to successfully scale up the related CFD simulations to an entire SMR core for the first time.

IMPACT

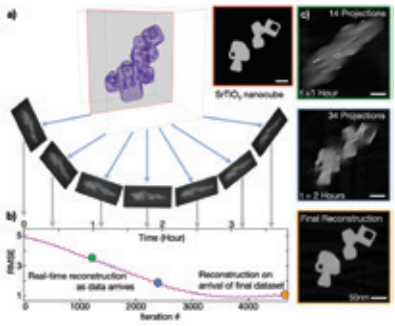
This work marks an important milestone on the path to the ultimate research objective of ExaSMR and permits development of novel momentum sources to model key core structures and providing information that can help reshape how we approach the challenges in reactor designs.

PUBLICATIONS

Fang, J., D. R. Shaver, A. Tomboulides, M. Min, P. Fischer, Y.-H. Lan, R. Rahaman, P. Romano, S. Benhamadouche, Y. A. Hassan, A. Kraus, and E. Merzari. "Feasibility of Full-Core Pin Resolved CFD Simulations of Small Modular Reactor with Momentum Sources," *Nuclear Engineering and Design* (April 2021), Elsevier.

Dynamic Compressed Sensing for Real-Time Tomographic Reconstruction

PI Robert Hovden, University of Michigan
AWARD ADSP
HOURS Theta: 10,000 Node-Hours



a) As the tomographic experiment progresses, projections are collected across an angular range. Measured projections are fed into the dynamic CS algorithm for 3D reconstruction. b) As the amount of data increases, the root mean square error (RMSE) decreases. c) 2D slices of the 3D reconstruction at various time stamps. *Image: Jonathan Schwartz, University of Michigan*

Electron and x-ray tomography allow researchers to perform 3D characterization of materials at the nano- and mesoscale, generating data that is critical to the development of nanomaterials for a wide range of applications, including solar cells and semiconductor devices. With an ALCF Data Science Program (ADSP) award, a University of Michigan-led research team is leveraging recent advancements in tomographic reconstruction algorithms, such as compressed sensing methods, to enhance and accelerate materials characterization research.

CHALLENGE

Compressed sensing algorithms provide higher quality reconstructions, but they require substantially more computation time to complete, causing the rapidly expanding field of tomography to become critically bottlenecked by low throughput. To address these challenges and achieve real-time tomographic reconstruction using compressed sensing algorithms, the ADSP team has developed a dynamic framework that performs in-situ reconstruction simultaneous to data collection.

APPROACH

With access to DOE supercomputing resources, the researchers are conducting comprehensive simulations for real-time electron tomography and developing reconstruction methods for through-focal tomography. The team is experimentally demonstrating their reconstruction workflow and methods on commercial scanning transmission electron microscopes and the ptychographic tomography instruments at Argonne's Advanced Photon Source (APS).

RESULTS

A paper published in *Microscopy and Microanalysis* demonstrated that multi-modal spectroscopy can substantially improve the quality of under-measured spectral maps and ensure accurate chemical recovery.

A paper published in the same journal demonstrated real-time tomography on a helical nanoparticle consisting of a Cysteine amino-acid coordinated with Cadmium. Real-time tomography enabled, via direct visualization of the specimen's 3D structure, immediate identification of morphological and internal information, with overall specimen morphology observed within five minutes and left-handed chirality discerned within 20 minutes; a high-resolution volume was available shortly thereafter when the experiment was 50 percent complete.

IMPACT

The team's approach will help advance materials characterization research by enabling real-time analysis of 3D specimens while an experiment progresses. By integrating their framework with an open-source 3D visualization and tomography software package, the team's techniques will be accessible to a wide range of researchers and enable new material characterizations across academia and industry.

PUBLICATIONS

Schwartz, J., C. Harris, J. Pietryga, H. Zheng, P. Kumar, A. Visheratina, N. Kotov, Y. Jiang, M. Hanwell, and R. Hovden. "Real-Time 3D Analysis During Tomographic Experiments on tomviz," *Microscopy and Microanalysis* (July 2021), Cambridge University Press.

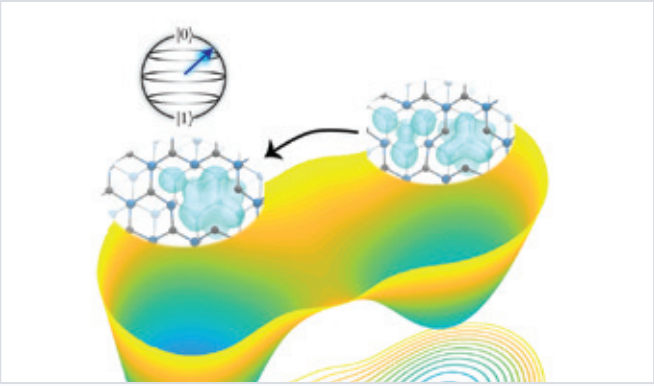
Materials Science | Simulation

Towards Automated Discovery and Optimization of Spin Defects for Quantum Technologies

PI Giulia Galli, Argonne National Laboratory and University of Chicago

AWARD INCITE

HOURS Theta: 1,200,000 Node-Hours



Pictorial representation of the free energy of defects in SiC, representing the formation of divacancies (left) from monovacancies (right). *Image: Elizabeth Lee, University of Chicago*

Spin defects in wide-bandgap semiconductors provide a promising platform for the creation of qubits, or quantum bits, the basic units of quantum information technologies. Their synthesis and optical characterization, however, present considerable challenges, and the mechanisms responsible for their generation or annihilation are poorly understood. Researchers at Argonne National Laboratory and the University of Chicago carried out atomistic and first-principles simulations to elucidate spin defect formation processes in silicon carbide (SiC) and developed a protocol, based on density functional theory calculations, to predict their photoluminescence spectra.

CHALLENGE

Understanding the formation of defects in semiconductors represents a challenge for both theory and experiments. The researchers focused here on the divacancy complex (VV) in SiC, a key candidate for qubits and investigated its formation process at the atomistic level, using atomistic and quantum simulations coupled with enhanced sampling methods, and density functional theory (DFT) electronic structure calculations.

APPROACH

Leveraging the Theta system to model silicon carbide at the atomistic scale, the researchers employed a combination of codes to study defects in this system. They carried out classical simulations with the LAMMPS code, and quantum simulations with the Qbox code coupled with the sampling suite of codes SSAGES; the positions of vacancy defects, on the other hand, were tracked using the VORO++ software library. They performed electronic structure calculations with both the Quantum Espresso and the Qbox codes. The research was carried out within the Midwest Integrated Center for Computational Materials.

RESULTS

As detailed in a paper published in *Nature Communications*, the researchers determined that the VV formation is a thermally activated process that competes with the conversion of silicon-to-carbon monovacancies, and that VV reorientation can occur without dissociation. Moreover, their work identified pathways for the creation of spin defects consisting of antisite-double-vacancy complexes, and determined their electronic properties—potentially facilitating the realization of qubits in industrially relevant materials.

IMPACT

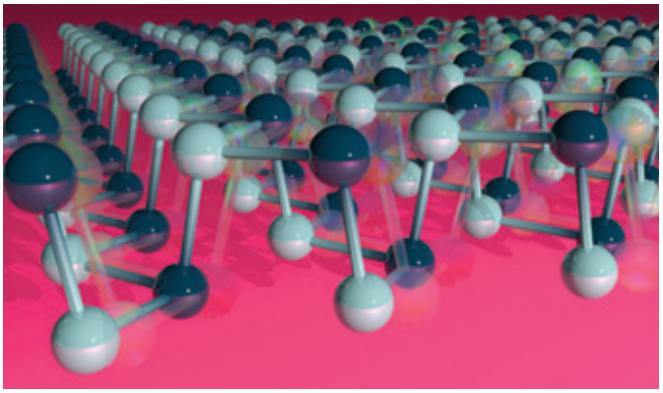
This work provides predictions of the structural and electronic properties of heterogeneous systems that further develop our understanding of how defective and nanostructured materials interact with light, as well as validated data for systems germane to sustainable and quantum technologies. Its research lays the foundation for an integrated experimental and theoretical strategy for the design and optimization of spin defects for quantum technologies.

PUBLICATIONS

Lee, E. M. Y., A. Yu, J. J. de Pablo, and G. Galli. "Stability and Molecular Pathways to the Formation of Spin Defects in Silicon Carbide," *Nature Communications* (November 2021), Springer Nature.

Towards Predictive Simulations of Functional and Quantum Materials

PI Paul Kent, Oak Ridge National Laboratory
AWARD INCITE
HOURS Theta: 1,500,000 Node-Hours



Optimized geometry of GeSe monolayer using the newly developed structural optimization algorithm within Quantum Monte Carlo (colored structure) compared to the initial Density Functional Theory optimized structure (clear structure). *Image: Janet Knowles, Joseph Insley, Silvio Rizzi, and Victor Mateevitsi, Argonne National Laboratory*

Given their unique properties and tunability, 2D semiconductor nanomaterials are good candidates for use in electronics and optical sensors. Newly developed quantum Monte Carlo (QMC) methods were used to find the structure and electronic band gap of one such material, germanium selenide (GeSe).

CHALLENGE

Considering the significant potential of 2D materials, researchers are greatly motivated to determine the properties of monolayer GeSe and how to calculate them. In bulk quantities this material forms a 3D layered structure with layers bonded by van der Waals interactions. Different density functional theory (DFT) results have yielded significantly varying geometries and band gaps.

APPROACH

High-accuracy many-body diffusion Monte Carlo (DMC) methods were used obtain an optimized GeSe structure and calculate the energy gaps of charged quasiparticle and neutral excitations. DMC was also used to verify the experimental structure and electronsic properties for bulk GeSe. A newly developed DMC structural optimization method was subsequently applied to monolayer GeSe; this method, based on a surrogate Hessian, is less computationally expensive costs than prior techniques. The researchers employed Theta for equation of state for bulk GeSe, bandgap calculations, and geometry optimization of the monolayer.

RESULTS

This work resulted in the first full structural relaxation of a periodic nanostructure using QMC. Indicating the strong tunability of monolayer GeSe's optical absorption properties, the DMC energy surface has a shallow minimum at the optimal structure, while the electronic properties vary strongly with strain: not only does the magnitude of the band gap change with strain, but strain can induce a transition from a direct to an indirect gap. The tunability may be a general feature of this class of materials. A multideterminant wavefunction method confirmed that potential sources of error in DMC calculations were small. The researchers also determined that no DFT exchange-correlation functional they tested could simultaneously yield both accurate band gaps and structure, demonstrating the importance of many-body methods such as DMC for mono- and few-layer van der Waals materials.

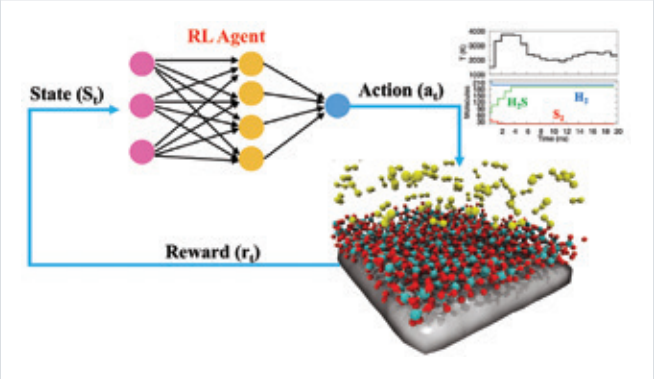
IMPACT

GeSe is considered a promising material for light-detecting devices such as solar cells and photodetectors. Highly accurate QMC methods were used to obtain the full geometry of a complex 2D nanomaterial for the first time. The newly developed QMC-based algorithm can accurately determine the structure of a material without calculating the atomic forces. The high tunability of the band gaps indicates potential optical applications in this class of materials. This work also clearly demonstrated the need for highly accurate structural and electronic structure methods to reliably assess the properties of these materials for use in future applications.

PUBLICATIONS
Shin, H., J. T. Krogel, K. Gasperich, P. R. C. Kent, A. Benali, and O. Heinonen. "Optimized Strucutre and Electronic Band Gap of Monolayer GeSE from Quantum Monte Carlo Methods," *Physical Review Materials* (February 2021), APS.

Ultrafast Control of Functional Materials

PI Priya Vashishta, University of Southern California
AWARD INCITE
HOURS Theta: 1,600,000 Node-Hours



Reinforcement-learning-assisted AI agent for MoS_2 synthesis by chemical vapor deposition. Here, the agent learns to propose optimal time-dependent synthesis conditions in terms of temperature and reactant gas concentration to create defect-free MoS_2 crystal with minimal human supervision. *Image: Pankaj Rajak, Argonne National Laboratory and University of Southern California*

Artificial intelligence (AI) methods, such as machine learning and neural networks, have shown great potential in accelerating the discovery of new functional materials. With this INCITE project, researchers from the University of Southern California are combining advanced AI techniques with leadership-scale quantum dynamics simulations and experimental data to extend the frontiers of computational materials science.

CHALLENGE

It can take 10–20 years or more to move a material from initial discovery to the market. This long timeline results from the empirical discovery of promising materials as well as the trial-and-error approach to identifying scalable synthesis routes for these material candidates. In recent years, an increase in available computing power and the enhanced efficiency of ab initio and AI-driven simulation software has helped accelerate large-scale computational materials screening by enabling high-throughput simulations of several tens of thousands of materials.

APPROACH

The INCITE team continues to expand the physics and chemistry that can be described by their two primary codes: QXMD, a non-adiabatic quantum molecular dynamics simulation engine; and RXMD, a reactive molecular dynamics simulation engine. They are also leveraging novel methods, such as deep neural networks and reinforcement learning (RL), to advance their research into a variety of materials. In addition, the team is benefitting from synergy between their INCITE project and a related Aurora Early Science Program project, which is helping to further improve the performance of their simulation engines on Theta.

RESULTS

Using ALCF computing resources, the researchers have carried out several studies to explore new computational methods for materials discovery and development. In a paper published in *Physical Review Letters*, the team employed two neural networks to investigate the dielectric constant and its temperature dependence for liquid water. Their scalable method, which is applicable to a range of different materials and systems, computed dielectric constants that were in good agreement with experimental data.

In addition, the team used RL for two separate studies published in *npj Computational Materials*. In one paper, researchers employed an autonomous RL agent to predict the optimal synthesis conditions for the 2D quantum material, MoS_2, using chemical vapor deposition. In the other study, they successfully applied RL to generate a wide range of highly stretchable MoS_2 kirigami structures from an extremely large search space consisting of millions of structures.

IMPACT

The team's use of emerging AI techniques is accelerating efforts to identify promising material compositions and phases. Ultimately, this research will help inform the discovery and synthesis of new materials engineered for targeted applications, such as batteries, catalysts, and solar cells.

PUBLICATIONS

Krishnamoorthy A., K. Nomura, N. Baradwaj, K. Shimamura, P. Rajak, A. Mishra, S. Fukushima, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. "Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics," *Physical Review Letters* (May 2021), APS.

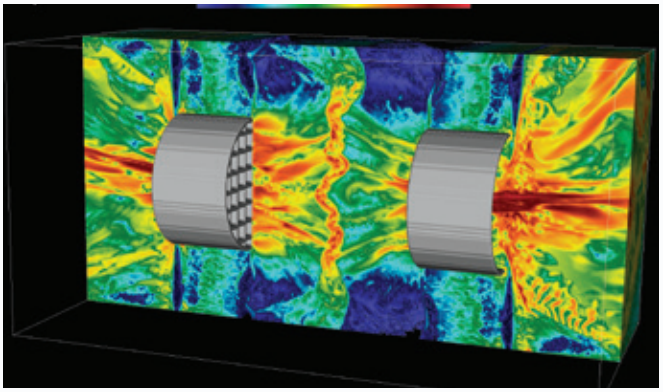
Rajak P., A. Krishnamoorthy, A. Mishra, R. Kalia, A. Nakano, and P. Vashishta. "Autonomous Reinforcement Learning Agent for Chemical Vapor Deposition Synthesis of Quantum Materials," *npj Computational Materials* (July 2021), Springer Nature.

Rajak P., B. Wang, K. Nomura, Y. Luo, A. Nakano, R. Kalia, and P. Vashishta. "Autonomous Reinforcement Learning Agent for Stretchable Kirigami Design of 2D Materials," *npj Computational Materials* (July 2021), APS.

Physics | Simulation

Amplification of Cosmic Magnetic Fields Captured in Laser Experiments

PI Petros Tzeferacos, University of Rochester
AWARD ALCC
HOURS Mira: 1,375,000 Node-Hours



FLASH simulation of the experiment showing the magnetic fields achieved. *Image: Petros Tzeferacos, University of Rochester*

The origin of cosmic magnetic fields that thread our universe is not fully understood. Astrophysicists believe that a key mechanism behind their origin is turbulent dynamo, a process by which stochastic motions amplify and sustain cosmic magnetic fields at the values we observe today. Although this physical process occurs readily in space, it is extremely hard to recreate and study in the laboratory. Researchers of the turbulent dynamo collaboration, an international team co-led by the University of Rochester and the University of Oxford performed laser experiments that captured—for the first time in the laboratory—the growth rate of magnetic fields by the turbulent dynamo mechanism, in conditions relevant to most astrophysical systems.

CHALLENGE

These laser-driven plasma experiments were able to reproduce experimentally turbulent dynamo and, for the first time in the laboratory, access the viscosity-dominated regime that is relevant to most plasmas in the universe. The scientists were also able, for the first time, to record time-resolved measurements of the properties of the mechanism, including the growth rate of the magnetic field, previously only available from simulations.

APPROACH

To design their experiments (conducted at the University of Rochester's Omega Laser Facility), the researchers leveraged Mira to construct a novel experimental platform using numerical simulations performed with FLASH, a publicly available simulation code that can accurately model laser-driven laboratory plasma experiments. The platform consists of a pair of plastic foils that are driven with twenty OMEGA laser beams. The laser ablation launches a pair of magnetized plasma flows that propagate through offset grids, and collide and shear to create a hot, turbulent plasma. The turbulent plasma achieves a regime where turbulent dynamo can amplify the advected seed magnetic fields to magnetic energies comparable to the kinetic energy of the stochastic motions.

RESULTS

As detailed in a paper published in Proceedings of the National Academy of Sciences, the researchers found rapid magnetic field amplification that exceeds theoretical expectations, a result that could help explain the origin of present-day large-scale fields observed in galaxy clusters.

IMPACT

The ability to recreate and study turbulent dynamo in the laboratory is a long-sought goal for physicists and astrophysicists. The properties of this fundamental mechanism were previously only available from simulations and analytical calculations. These experiments now provide strict constraints to existing models and help explain astronomical measurements. The efficient amplification of magnetic fields at large scales seen in the experiments could explain the origin of large-scale fields observed in galaxy clusters, which are not predicted by current idealized simulations. These experiments answer key astrophysics questions and establish laboratory experiments as a component in the study of turbulent dynamo.

PUBLICATIONS

Bott, A. F. A., P. Tzeferacos, L. Chen, C. A. J. Palmer, A. Rigby, A. R. Bell, R. Bingham, A. Birkel, C. Graziani, D, H. Froula, J. Katz, M. Koenig, M. W. Kunz, C. Li, J. Meinecke, F. Miniati, R. Petrasso, H.-S. Park, B. A. Remington, B. Reville, J. S. Ross, D. Ryu, D. Ryutov, F. H. Séguin, T. G. White, A. A. Schekochihin, D. Q. Lamb, and G. Gregori. "Time-Resolved Turbulent Dynamo in a Laser Plasma," *Proceedings of the National Academy of Sciences* (March 2021), National Academy of Sciences.

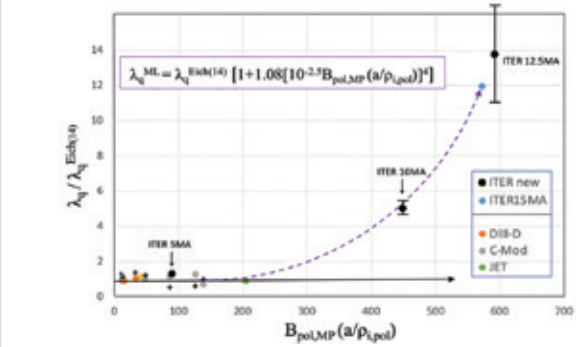
Physics | Simulation, Learning

High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics

PI Choong-Seock Chang,
Princeton Plasma Physics Laboratory

AWARD INCITE

HOURS Theta: 1,500,000 Node-Hours



A supervised machine-learning program finds a hidden kinetic parameter. Three more ITER simulations (black symbols) have been performed to verify the validity of the new ML-found formula (black dots). *Image: C. S. Chang, Princeton Plasma Physics Laboratory*

This multi-year INCITE project seeks to advance our understanding of the edge plasma physics in fusion reactors, with a focus on ITER, and to assemble a burning plasma experiment that can demonstrate the scientific and technological feasibility of fusion.

CHALLENGE

The INCITE team is performing studies on two high-priority challenges: (1) quantifying the narrowness of the heat-flux width on the ITER divertor material plates in the high-confinement mode (H-mode) operation during tenfold energy gain operation; and (2) understanding the basic physics behind the low-to-high mode L-H transition and pedestal formation at the edge, which is necessary to achieve a tenfold energy gain in ITER.

APPROACH

The researchers are using the 5D gyrokinetic particle code, XGC, on DOE leadership computing resources to address some of the most difficult plasma physics questions facing ITER. The team used this extreme-scale modeling code to solve kinetic equations for the tokamak edge by modeling plasma with a large number of particles. Predictions from XGC for the divertor heat-load width on present tokamaks agreed with experimental data within the experimental error bar, yielding narrower divertor heat-loads than what are hoped for. To find the hidden parameters, the team used a supervised machine-learning program to anchor, or direct, the extrapolation from the existing tokamak data to the future ITER data obtained from the XGC high-fidelity kinetic simulation.

RESULTS

The teams' findings were published in *Physics of Plasma*. A simple extrapolation to full-power ITER would give a pessimistically narrow divertor heat-load width. However, when the same XGC code was applied to the full-power ITER, it produced a divertor heat-load width more than six times greater than predicted by the formulas developed from a simple data extrapolation from present tokamaks. The surprising result was subsequently confirmed by increasing the model of particles to trillions while running on Summit at OLCF. The new predictive formula has been successfully verified by simulating lower-power ITER plasmas on Theta.

IMPACT

Understanding and predicting divertor heat-load width is critically important for robust ITER operation. Establishing an accurate predictive formula for the exhaust heat-load width of future doughnut-shaped tokamak fusion reactors can help enable researchers to progress faster toward the goal of 0.5 GW of fusion power production from 50 MW of input power. A more accurate formula can also help inform more reliable designs for future fusion reactors, which currently suffer from the limitation imposed by exhaust heat-load width on the divertor plates.

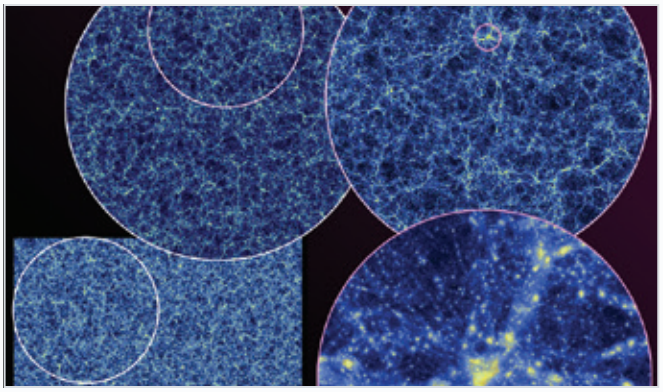
PUBLICATIONS

Chang C. S., S. Ku, R. Hager, R. M. Churchill, J. Hughes, F. Köchl, A. Loarte, V. Parail, and R. A. Pitts. "Constructing a New Predictive Scaling Formula for ITER's Divertor Heat-Load Width Informed by a Simulation-Anchored Machine Learning," *Physics of Plasma* (February 2021), AIP Publishing.

Physics | Simulation

Mira's Last Journey

PI Katrin Heitmann, Argonne National Laboratory
AWARD ALCC
HOURS Mira: 50,000,000 Node-Hours



Dark-matter-dominated halos from a small region of the simulation. The radius of the spheres is proportional to halo mass; the dominant halo is the simulation's largest, at ~6 x 1015 solar masses. *Image: ALCF Visualization and Data Analysis Team and the HACC Team*

This project, led by Argonne National Laboratory researchers, is among the world's largest cosmological simulations to attain sufficient resolution and volume to permit the generation of detailed sky maps across multiple wavebands that are targeted towards upcoming cosmological surveys. Running on the entirety of the Mira system, the simulation modeled the lifespan of the universe to help answer some of science's deepest questions.

CHALLENGE

The research team structured the simulation to begin 50 million years after the Big Bang, with conditions that agree with the most up-to-date cosmological observations. Billions of years of evolution between then and now were subsequently modeled in order to create a high-resolution model of what a large portion of the universe should look at present day. Running on the full machine generated such a massive quantity of data that it posed the additional challenge of requiring significant on-the-fly analysis.

APPROACH

The project was implemented using the Hardware/Hybrid Accelerated Cosmology Code (HACC) simulation and analysis framework on the full Mira system. The simulation evolved more than 1.24 trillion particles to resolve the cosmological structures which host faint galaxies that will be observed by the Legacy Survey of Space and Time (LSST) project when it is carried out at the Vera Rubin Observatory. Cosmological parameters chosen to be consistent with the results from the Planck satellite. Analysis outputs were generated such that synthetic galaxy catalogs could be constructed using a semi-analytic modeling approach in post-processing.

RESULTS

The detailed history of the evolution of cosmological structures is now being processed to create synthetic sky maps for optical and cosmic microwave background surveys. Initial results have been documented in a sequence of papers published in *The Astrophysical Journal Supplement Series*. As part of their in-situ analysis pipeline, the researchers employed a new method for tracking halo substructures, introducing the concept of subhalo structures.

IMPACT

This simulation was designed to address numerous fundamental questions in cosmology; the data produced are essential for enabling the refinement of existing predictive tools and aid the development of new models, impacting both ongoing and upcoming cosmological surveys, including the Dark Energy Spectroscopic Instrument (DESI), the LSST, SPHEREx, and the "Stage-4" ground-based cosmic microwave background experiment (CMB-S4).

PUBLICATIONS

Heitmann, K., N. Frontiere, E. Rangel, P. Larsen, A. Pope, I. Sultan, T. Uram, S. Habib, H. Finkel, D. Korytov, E. Kovacs, S. Rizzi, and J. Insley. "The Last Journey. I. An Extreme-Scale Simulation on the Mira Supercomputer," *The Astrophysical Journal Supplement Series* (January 2021), IOP Publishing.

Sultan, I., N. Frontiere, S. Habib, K. Heitmann, E. Kovacs, P. Larsen, and E. Rangel. "The Last Journey. II. SMACC—Subhalo Mass-loss Analysis Using Core Catalogs," *The Astrophysical Journal* (June 2021), IOP Publishing.

ALCF Projects

INCITE 2021

CHEMISTRY

Design of Peptides and Proteins on Classical and Quantum Computing Hardware

PI Vikram Mulligan, Flatiron Institute
HOURS ALCF: 800,000 Node-Hours

EARTH SCIENCE

Energy Exascale Earth System Model

PI Mark Taylor, Sandia National Laboratories
HOURS ALCF: 1,800,000 Node-Hours
OLCF: 1,000,000 Node-Hours

Extreme-Scale Simulations for Advanced Seismic Ground Motion and Hazard Modeling

PI Christine Goulet, University of Southern California
HOURS ALCF: 480,000 Node-Hours
OLCF: 319,000 Node-Hours

ENERGY TECHNOLOGIES

DNS and LES of Internal Combustion Engines to Understand Origins of CCV

PI Sibendu Som, Argonne National Laboratory
HOURS ALCF: 1,000,000 Node-Hours

ENGINEERING

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

PI Kenneth Jansen, University of Colorado Boulder
HOURS ALCF: 1,000,000 Node-Hours

High-Speed Turbulence with Shocks over Non-Adiabatic and Flexible Walls

PI Johan Larsson, University of Maryland
HOURS ALCF: 1,800,000 Node-Hours

MATERIALS SCIENCE

First-Principles Simulation of Electronic Stopping Excitation and Beyond

PI Yosuke Kanai, University of North Carolina at Chapel Hill
HOURS ALCF: 1,900,000 Node-Hours

Large-Scale Simulations of Light-Activated Matter

PI Giulia Galli, University of Chicago and Argonne National Laboratory
HOURS ALCF: 1,200,000 Node-Hours

Predicting Ion Transport Kinetics at Complex Interfaces for Energy Storage

PI Brandon Wood, Lawrence Livermore National Laboratory
HOURS ALCF: 640,000 Node-Hours

Towards a Definitive Model of Core-Collapse Supernova Explosions

PI Adam Burrows, Princeton University
HOURS ALCF: 2,000,000 Node-Hours

Towards Predictive Simulations of Functional and Quantum Materials

PI Paul Kent, Oak Ridge National Laboratory
HOURS ALCF: 1,800,000 Node-Hours
OLCF: 500,000 Node-Hours

Ultrafast Control of Functional Materials

PI Priya Vashishta, University of Southern California
HOURS ALCF: 1,600,000 Node-Hours

PHYSICS

Ab-initio Nuclear Structure and Nuclear Reactions

PI Gaute Hagen, Oak Ridge National Laboratory
HOURS ALCF: 500,000 Node-Hours
OLCF: 693,000 Node-Hours

High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics

PI Choongseock Chang, Princeton Plasma Physics Laboratory
HOURS ALCF: 1,300,000 Node-Hours
OLCF: 900,000 Node-Hours

Petascale Simulations of Kinetic Effects in IFE Plasmas

PI Frank Tsung, University of California, Los Angeles
HOURS ALCF: 1,800,000 Node-Hours
OLCF: 900,000 Node-Hours

Towards a Definitive Model of Core-Collapse Supernova Explosions

PI Adam Burrows, Princeton University
HOURS Theta: 2,000,000 Node-Hours

ALCC 2020–2021

COMPUTER SCIENCE

Enabling Resilient and Portable Workflows from DOE's Experimental Facilities

PI Katie Antypas, Lawrence Berkeley National Laboratory
HOURS ALCF: 100,000 Node-Hours
OLCF: 20,000 Node-Hours

CHEMISTRY

Benchmarking Many-Body Perturbation Theory

PI Olle Heinonen, Argonne National Laboratory
HOURS ALCF: 100,000 Node-Hours

Interpretable Machine Learning Force Fields for Accurate Chemical Reactive Dynamic

PI Olexandr Isayev, Carnegie Mellon University
HOURS ALCF: 359,000 Node-Hours

Stochastic A Priori Dynamics for Complex Reactive Chemical Environments

PI Ahren Jasper, Argonne National Laboratory
HOURS ALCF: 100,000 Node-Hours

Understanding the Role of Hierarchical Correlations in Solution-Phase Chemical Separations

PI Lynda Soderholm, Argonne National Laboratory
HOURS ALCF: 100,000 Node-Hours

EARTH SCIENCE

Variable-Resolution Earth System Modeling of the Cryosphere with E3SM

PI Darin Comeau, Los Alamos National Laboratory
HOURS ALCF: 400,000 Node-Hours
NERSC: 500,000 Node-Hours

ENERGY TECHNOLOGIES

Automatic Building Energy Modeling

PI Joshua New, Oak Ridge National Laboratory
HOURS ALCF: 300,000 Node-Hours

DNS Simulations of Coolant Flow in the High-Flux Isotope Reactor

PI Emilian Popov, Oak Ridge National Laboratory
HOURS ALCF: 220,000 Node-Hours

Multiphase Flow Simulations of Reactor Flows

PI Igor Bolotnov, North Carolina State University
HOURS ALCF: 192,000 Node-Hours
NERSC: 250,000 Node-Hours

Toward the Future: High-Fidelity Simulation for Next-Generation Nuclear Reactors

PI Yiqi Yu, Argonne National Laboratory
HOURS ALCF: 208,000 Node-Hours
NERSC: 300,000 Node-Hours

MATERIALS SCIENCE

Data-Driven Molecular Engineering of Advanced Functional Materials

PI Jacqueline Cole, University of Cambridge
HOURS ALCF: 100,000 Node-Hours

High-Temperature Material Properties from First Principles

PI Mark Messner, Argonne National Laboratory
HOURS ALCF: 200,000 Node-Hours

Many-Body Perturbation Theory Meets Machine Learning to Discover Materials for Organic Photovoltaics

PI Noa Marom, Carnegie Mellon University
HOURS ALCF: 100,000 Node-Hours

Plasma Surface Interaction Modeling

PI Brian Wirth, University of Tennessee
HOURS ALCF: 318,000 Node-Hours
OLCF: 155,000 Node-Hours
NERSC: 30,000 Node-Hours

Predictive Modeling of Nanoporous Materials and Multiphase Systems

PI Joern Siepmann, University of Minnesota
HOURS ALCF: 220,000 Node-Hours

Supercomputing for Automotive High-Temperature Alloy Design

PI Dongwon Shin, Oak Ridge National Laboratory
HOURS ALCF: 100,000 Node-Hours

PHYSICS

Reconstructing Neutrino Data with the MicroBooNE Liquid Argon Detector

PI Andrzej Szelc, University of Manchester
HOURS ALCF: 200,000 Node-Hours

Optimization Studies of the LBNF - PIP-II Complex for Megawatt Beams on Target

PI Igor Rakhno, Fermi National Accelerator Laboratory
HOURS ALCF: 450,000 Node-Hours

Chiral Nuclear Interactions from Nuclei to Nucleonic Matter

PI Maria Piarulli, Washington University in St. Louis
HOURS ALCF: 200,000 Node-Hours

Nucleon Axial Charge with All-Staggered Lattice QCD

PI Andreas Kronfeld, Fermi National Accelerator Laboratory
HOURS ALCF: 200,000 Node-Hours
NERSC: 870,000 Node-Hours

Distributed Large Wavefield Propagation and 3D Reconstruction Beyond the Depth of Focus Limit

PI Ming Du, Argonne National Laboratory
HOURS ALCF: 250,000 Node-Hours

Field-Reversed Configuration Stability and Transport

PI Sean Dettrick, TAE Technologies Inc.
HOURS ALCF: 64,000 Node-Hours

Improving Direct-Drive Laser Fusion Predictive Capability with a Simulation Database

PI Duc Cao, Laboratory for Laser Energetics
HOURS ALCF: 318,000 Node-Hours

Improving Direct-Drive Laser Fusion Predictive Capability with a Simulation Database

PI Duc Cao, Laboratory for Laser Energetics
HOURS ALCF: 318,000 Node-Hours

High-Luminosity LHC Detector Upgrade Studies by the ATLAS and CMS Collaborations

PI Douglas Benjamin, Argonne National Laboratory
HOURS ALCF: 950,000 Node-Hours

ALCC 2021–2022

BIOLOGICAL SCIENCES

Probabilistic Comparative Modeling of Colorectal Cancer Screening Strategies

PI Jonathan Ozik, Argonne National Laboratory
HOURS ALCF: 160,000 Node-Hours

CHEMISTRY

Microscopic Insight Into Transport Properties of Li-Battery Electrolytes

PI Wei Jiang, Argonne National Laboratory
HOURS ALCF: 1,032,000 Node-Hours

Multimodal Imaging with Intense X-ray Pulses

PI Phay Ho, Argonne National Laboratory
HOURS ALCF: 316,000 Node-Hours

EARTH SCIENCE

Advancing Multi-Year to Decadal Climate Prediction with High-Resolution E3SM and CESM

PI Ben Kirtman, University of Miami
HOURS ALCF: 1,000,000 Node-Hours

Improving the Representation of Mesoscale Convective Systems in Weather and Climate

PI Andreas Prein, National Center for Atmospheric Research
HOURS ALCF: 372,000 Node-Hours

Multi-Decadal, Climate-Scale Convection-Resolving Simulations for North America

PI V. Rao Kotamarthi, Argonne National Laboratory
HOURS ALCF: 300,000 Node-Hours

Multi-Scale Multi-Physics Ensemble Simulations for Aerosol-Cloud Interactions

PI Po-Lun Ma, Pacific Northwest National Laboratory
HOURS ALCF: 400,000 Node-Hours

ENERGY TECHNOLOGIES

Cavitation Dynamics in the Spallation Neutron Source Target

PI Eric Johnsen, University of Michigan
HOURS ALCF: 108,000 Node-Hours
OLCF: 4,000 Node-Hours

High-Fidelity CFD Simulations Supporting the Needs of Industry and the DOE

PI Dillon Shaver, Argonne National Laboratory
HOURS ALCF: 550,000 Node-Hours
OLCF: 80,000 Node-Hours

High-Fidelity Physics Simulations for DOE and Industry Fast Spectrum Nuclear Reactor Systems

PI Emily Shemon, Argonne National Laboratory
HOURS ALCF: 880,000 Node-Hours

High-Fidelity Simulation of Flow and Heat Transfer Behavior to Support Conversion of Research Reactors with Involute Shaped Fuel Elements to Low Enriched Uranium

PI Yiqi Yu, Argonne National Laboratory
HOURS ALCF: 500,000 Node-Hours

ENGINEERING

Multiscale Bubble Breakup and Gas Transfer in Turbulent Oceanic Environments

PI Parviz Moin, Stanford University
HOURS ALCF: 650,000 Node-Hours
NERSC: 500,000 Node-Hours

MATERIALS SCIENCE

Inverse Design of Multicomponent Oxide Catalysts with Generative Models and DFT

PI Rafael Gomez-Bombarelli, Massachusetts Institute of Technology
HOURS ALCF: 400,000 Node-Hours
OLCF: 50,000 Node-Hours
NERSC: 200,000 Node-Hours

Modeling of Polymeric Materials for Energy Storage Across Scales

PI Juan de Pablo, University of Chicago
HOURS ALCF: 100,000 Node-Hours

Response Functions of LaNiO2: Insights into High-Temperature Superconductivity

PI Gabriel Kotliar, Rutgers University
HOURS ALCF: 115,000 Node-Hours

PHYSICS

AI/Deep Learning Prediction & Real-Time Control for Fusion Energy Systems

PI William Tang, Princeton University
HOURS ALCF: 45,000 Node-Hours

LBNF - PIP-II Optimization Studies for Megawatt 120-GeV Beams on Target

PI Igor Rakhno, Fermi National Accelerator Laboratory
HOURS ALCF: 450,000 Node-Hours

Quantum Monte Carlo Calculations of Nuclei Up to 16O and Neutron matter

PI Alessandro Lovato, Argonne National Laboratory
HOURS ALCF: 632,000 Node-Hours

ALCF DATA SCIENCE PROGRAM

Advanced Materials Characterization with AI-Informed Computation

PI Marco Govoni, Argonne National Laboratory

Autonomous Molecular Design for Redox Flow Batteries

PI Logan Ward, Argonne National Laboratory

Deep Learning at Scale for Multimessenger Astrophysics Through the NCSA-Argonne Collaboration

PI Eliu Huerta, University of Illinois at Urbana-Champaign

Developing High-Performance-Computing Applications for Liquid Argon Neutrino Detectors

PI Andrzej Szelc, The University of Manchester

Dynamic Compressed Sensing for Real-Time Tomographic Reconstruction

PI Robert Hovden, University of Michigan

Learning Optimal Image Representations for Current and Future Sky Surveys

PI George Stein, Lawrence Berkeley National Laboratory

Machine Learning for Data Reconstruction to Accelerate Physics Discoveries in Accelerator-Based Neutrino Oscillation Experiments

PI Marco Del Tutto, Fermi National Accelerator Laboratory

Machine Learning Magnetic Properties of Van Der Waals Heterostructures

PI Trevor Rhone, Rensselaer Polytechnic Institute

X-ray Microscopy of Extended 3D Objects: Scaling Towards the Future

PI Chris Jacobsen, Argonne National Laboratory and Northwestern University

AURORA EARLY SCIENCE PROGRAM

Accelerated Deep Learning Discovery in Fusion Energy Science

PI William Tang, Princeton Plasma Physics Laboratory

Dark Sky Mining

PI Salman Habib, Argonne National Laboratory

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics

PI Kenneth Jansen, University of Colorado Boulder

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

PI Nicola Ferrier, Argonne National Laboratory

Exascale Computational Catalysis

PI David Bross, Argonne National Laboratory

Extending Moore's Law Computing with Quantum Monte Carlo

PI Anouar Benali, Argonne National Laboratory

Extreme-Scale Cosmological Hydrodynamics

PI Katrin Heitmann, Argonne National Laboratory

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

PI Amanda Randles, Duke University and Oak Ridge National Laboratory

Extreme-Scale Unstructured Adaptive CFD

PI Kenneth Jansen, University of Colorado Boulder

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas

PI C.S. Chang, Princeton Plasma Physics Laboratory

Machine Learning for Lattice Quantum Chromodynamics

PI William Detmold, Massachusetts Institute of Technology

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

PI Noa Marom, Carnegie Mellon University

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

PI Theresa Windus, Iowa State University and Ames Laboratory

Simulating and Learning in the ATLAS Detector at the Exascale

PI Walter Hopkins, Argonne National Laboratory

Virtual Drug Response Prediction

PI Rick Stevens, Argonne National Laboratory

2021 DIRECTOR'S DISCRETIONARY

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

BIOLOGICAL SCIENCES

AI-Driven Drug Discovery for SARS-CoV-2 Proteome

PI Arvind Ramanathan, Argonne National Laboratory

COVID-19 Spread and Effectiveness of Interventions

PI Jonathan Ozik, Argonne National Laboratory

Finding Druggable Sites in SARS-CoV-2 Proteins Using Molecular Dynamics and Machine Learning

PI Albert Lau, John Hopkins School of Medicine

Modeling Coronavirus

PI Zhangli Peng, University of Illinois at Chicago

Real-Time Analysis of SARS-CoV-2 Proteins

PI Darren Sherrell, Argonne National Laboratory

Simulation of Viral Infection Propagation Through Air-Travel

PI Ashok Srinivasan, University of West Florida

CHEMISTRY

Enantioselectivity in Heterogeneous Catalysts via the Addition of Chiral Modifiers

PI Wilfred T. Tysoe, University of Wisconsin-Milwaukee

Simulation of Industrial Flares

PI Marc Cremer, Reaction Engineering International

COMPUTER SCIENCE

DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications

PI Huihuo Zheng and Venkatram Vishwanath, Argonne National Laboratory

MPICH - A High Performance and Widely Portable MPI Implementation

PI Ken Raffenetti, Argonne National Laboratory

Rendezvous Algorithms for Large-Scale Modeling and Simulation

PI Steven Plimpton, Sandia National Laboratories

EARTH SCIENCE

Generation of a Next-Level Dataset for Regional Scale Climate Modeling: Convective Resolving Spatial Scales

PI Jiali Wang, Argonne National Laboratory

Using ARM Observations to Evaluate Process-Interactions in MCS Simulations Across Scales

PI Andreas Franz Prein, National Center for Atmospheric Research

ENERGY TECHNOLOGIES

Automatic Building Energy Modeling and Analysis

PI Joshua New, Oak Ridge National Laboratory

Cask Mis-Loads Evaluation Techniques

PI Angela Di Fulvio, University of Illinois at Urbana-Champaign

High-Fidelity CFD Simulations of Multi-Mode Combustion

PI Pinaki Pal, Argonne National Laboratory

LES Simulations of Severe Accident Conditions in Nuclear Containment

PI Christopher Boyd, Westinghouse Electric Company

ENGINEERING

Nek5000/NekRS for COVID Particle Transport and NRC

PI Aleksandr V. Obabko, Argonne National Laboratory

Towards Reactive DNS in Complex Internal Combustion Engine Geometries

PI Christos Frouzakis, ETH Zurich

MATERIALS SCIENCE

Designing Catalysts under Realistic Operating Conditions from the Atomic Scale

PI Hendrik Heinz, University of Colorado Boulder

Materials Informatics Study of Two-Dimensional Magnetic Materials and Their Heterostructures

PI Trevor Rhone, Rensselaer Polytechnic Institute

Structure and Properties of Grain Boundaries in Materials for Energy Applications

PI Wissam A Saidi, University of Pittsburgh

PHYSICS

Experimentally Driven Automated Machine-Learned Interatomic Potential for a Refractory Oxide

PI Ganesh Sivaraman, Argonne National Laboratory

LatticeQCD: Exascale Lattice Gauge Theory Opportunities/Requirements for Nuclear & High Energy Physics

PI Andreas Kronfeld, Fermilab

ALCF Publications

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

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

January

Koszorus, A., X. F. Yang, W. G. Jiang, S. J. Novario, S. W. Bai, J. Billowes, C. L. Binnersley, M. L. Bissell, T. E. Cocolios, B. S. Cooper, R. P. de Groote, A. Ekstrom, K. T. Flanagan, C. Forssen, S. Franchoo, R. F. Garcia Ruiz, F. P. Gustafsson, G. Hagen, G. R. Jansen, A. Kanellakopoulos, M. Kortelainen, W. Nazarewicz, G. Neyens, T. Papenbrock, P.-G. Reinhard, C. M. Ricketts, B. K. Sahoo, A. R. Vernon and S. G. Wilkins. "Charge Radii of Exotic Potassium Isotopes Challenge Nuclear Theory and the Magic Character of N = 32," *Nature Physics* (January 2021), Springer Nature. doi: 10.1038/s41567-020-01136-5

Garrison, E., and J. New. "Quality Control Methods for Advanced Metering Infrastructure Data," *Smart Cities* (January 2021), MDPI. doi: 10.3390/smartcities4010012

Sun, G., J. T. Fuller III, A. N. Alexandrova, and P. Sautet. "Global Activity Search Uncovers Reaction Induced Concomitant Catalyst Restructuring for Alkane Dissociation on Model Pt Catalysts," *ACS Catalysis* (January 2021), ACS Publications. doi: 10.1038/s41567-021-01253-9

Bieniek, M. K., A. P. Bhati, S. Wan, and P. V. Coveney. "TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing," *Journal of Chemical Theory and Computation* (January 2021), ACS Publications. doi: 10.1021/acs.jctc.0c01179

Quere, F., and H. Vincenti. "Reflecting Petawatt Lasers off Relativistic Plasma Mirrors: A Realistic Path to the Schwinger Limit," *High Power Laser Science and Engineering* (January 2021), Cambridge University Press. doi: 10.1017/hpl.2020.46

Ma, Y., S. E. Hoff, X. Huang, J. Liu, Q. Wan, Q. Song, J. Gu, H. Heinz, F. R. Tay, and L. Niu. "Involvement of Prenucleation Clusters in Calcium Phosphate Mineralization of Collagen," *Acta Biomaterialia* (January 2021), Elsevier. doi: 10.1016/j.actbio.2020.07.038

Benoit, A., V. Le Fevre, P. Raghavan, Y. Robert, and H. Sun. "Resilient Scheduling Heuristics for Rigid Parallel Jobs," *International Journal of Networking and Computing* (January 2021), IJNC Editorial Committee. doi: 10.15803/ijnc.11.1_2

Abram, G., F. Samsel, M. R. Petersen, X. Asay-Davis, D. Comeau, S. F. Price, and M. Potel. "Antarctic Water Masses and Ice Shelves: Visualizing the Physics," *IEEE Computer Graphics and Applications* (January 2021), IEEE. doi: 10.1109/MCG.2020.3044228

Britz, A., A. R. Attar, X. Zhang, H.-T. Chang, C. Nyby, A. Krishnamoorthy, S. H. Park, S. Kwon, M. Kim, D. Nordlund, S. Sainio, T. F. Heinz, S. R. Leone, A. M. Lindenberg, A. Nakano, P. Ajayan, P. Vashishta, D. Fritz, M.-F. Lin, and U. Bergmann. "Carrier-Specific Dynamics in 2H-MoTe2 Observed by Femtosecond Soft X-ray Absorption Spectroscopy Using an X-ray Free-Electron Laser," *Structural Dynamics* (January 2021), AIP. doi: 10.1063/4.0000048

Deng, G.-H, Y. Qian, T. Zhang, J. Han, H. Chen, and Y. Rao. "Two-Dimensional Electronic-Vibrational Sum Frequency Spectroscopy for Interactions of Electronic and Nuclear Motions at Interfaces," *PNAS* (January 2021), National Academy of Sciences. doi: 10.1073/pnas.2100608118

Wei, W., A. Khan, E. A. Huerta, X. Huang, and M. Tian. "Deep Learning Ensemble for Real-Time Gravitational Wave Detection of Spinning Binary Black Hole Mergers," *Physics Letters B* (January 2021), Elsevier. doi: 10.1016/j.physletb.2020.136029

Mallick, T., P. Balaprakash, E. Rask, and J. Macfarlane. "Transfer Learning with Graph Neural Networks for Short-Term Highway Traffic Forecasting," *25th International Conference on Pattern Recognition* (January 2021), IEEE. doi:10.1109/icpr48806.2021.9413270

Burrows, A., and D. Vartanyan. "Core-Collapse Supernova Explosion Theory," *Nature* (January 2021), Springer Science and Business Media. doi: 10.1038/s41586-020-03059-w

Milner, K. R., B. E. Shaw, C. A. Goulet, K. B. Richards-Dinger, S. Callaghan, T. H. Jordan, J. H. Dieterich, and E. H. Field. “Toward Physics-Based Nonergodic PSHA: A Prototype Fully Deterministic Seismic Hazard Model for Southern California,” *Bulletin of the Seismological Society of America* (January 2021), GeoScience World. doi: 10.1785/0120200216

Hoy, J. F., and I. Bermejo-Moreno. “Numerical Study of STBLI on Flexible Panels with Wall-Modeled LES,” *AIAA Scitech 2021 Forum* (January 2021), AAIA. doi: 10.2514/6.2021-0250

Wright, J. R., R. Balin, K. E. Jansen, and J. A. Evans. “Unstructured LES_DNS of a Turbulent Boundary Layer over a Gaussian Bump,” *AIAA Scitech 2021 Forum* (January 2021), AAIA. doi: 10.2514/6.2021-1746

Nagakura, H., A. Burrows, D. Vartanyan, and D. Radice. “Core-Collapse Supernova Neutrino Emission and Detection Informed by State-of-the-Art Three-Dimensional Numerical Models,” *Monthly Notices of the Royal Astronomical Society* (January 2021), Oxford University Press. doi: 10.1093/mnras/staa2691

Du, M., S. Kandel, J. Deng, X. Huang, A. Demortiere, T. T. Nguyen, R. Tucoulou, V. De Andrade, Q. Jin, and C. Jacobsen. “Adorym: A Multi-Platform Generic X-ray Image Reconstruction Framework based on Automatic Differentiation,” *Optics Express* (January 2021), Optica Publishing Group. doi: 10.1364/OE.418296

Nazarova, A. L., L. Yang, K. Liu, A. Mishra, R. K. Kalia, K. Nomura, A. Nakano, P. Vashishta, and P. Rajak. “Dielectric Polymer Property Prediction Using Recurrent Neural Networks with Optimizations,” *Journal of Chemical Information and Modeling* (January 2021), ACS. doi: 10.1021/acs.jcim.0c01366

Cruz-Torres, R., D. Lonardoni, R. Weiss, M. Piarulli, N. Barnea, D. W. Higinbotham, E. Piasetzky, A. Schmidt, L. B. Weinstein, R. B. Wiringa, and O. Hen. “Many-Body Factorization and Position–Momentum Equivalence of Nuclear Short-Range Correlations,” *Nature Physics* (January 2021), Springer Nature. doi: 10.1038/s41567-020-01053-7

Li, Y., A. Eshein, R. Virk, A. Eid, W. Wu, J. Frederick, D. VanDerway, S. Gladstein, K. Huang, A. R. Shim, N. M. Anthony, G. M. Bauer, X. Zhou, V. Agrawal, E. M. Pujadas, S. Jain, G. Esteve, J. E. Chandler, T.-Q. Nguyen, R. Bleher, J. J. de Pablo, I. Szleifer, V. P. Dravid, L. M. Almassalha, and V. Backman. “Nanoscale Chromatin Imaging and Analysis Platform Bridges 4D Chromatin Organization with Molecular Function,” Science Advances (January 2021), AAAS. doi: 10.1126/sciadv.abe4310

Li, Z., R. Chard, L. Ward, K. Chard, T. J. Skluzacek, Y. Babuji, A. Woodard, S. Tuecke, B. Blaiszik, M. J. Franklin, and I. Foster. “DLHub: Simplifying Publication, Discovery, and Use of Machine Learning Models in Science,” *Journal of Parallel and Distributed Computing* (January 2021), Elsevier. doi: 10.1016/j.jpdc.2020.08.006

Plimpton, S. J., and C. Knight. “Rendezvous Algorithms for Large-Scale Modeling and Simulation,” *Journal of Parallel and Distributed Computing* (January 2021), Elsevier. doi: 10.1016/j.jpdc.2020.09.001

Dong, G., K. G. Felker, A. Svyatkovskiy, W. Tang, and J. Kates-Harbeck. “Fully Convolutional Spatio-Temporal Models for Representation Learning in Plasma Science,” *Journal of Machine Learning for Modeling and Computing* (January 2021), Begell House. doi: 10.1615/jmachlearnmodelcomput.2021037052

Kanhaiya, K., S. Kim, W. Im, and H. Heinz. “Accurate Simulation of Surfaces and Interfaces of Ten FCC Metals and Steel Using Lennard-Jones Potentials,” *NPJ Computational Materials* (January 2021), Springer Nature. doi: 10.1038/s41524-020-00478-1

Lindquist, N., M. Min, and P. Fischer. “Scalable Interpolation on GPUs for Thermal Fluids Applications,” *Argonne Technical Report* (January 2021), OSTI. doi: 10.2172/1823469

February

Deshpande, A. S., and J. Poggie. “Large-Scale Unsteadiness in a Compression Ramp Flow Confined by Sidewalls,” *Physical Review Fluids* (February 2021), APS. doi: 10.1103/PhysRevFluids.6.024610

Rajak, P., A. Nakano, P. Vashishta, and R. Kalia. “Mechanical Behavior of Ultralight Nickel Metamaterial,” *Applied Physics Letters* (February 2021), AIP. doi: 10.1063/5.0031806

Hoja, J., L. Medrano Sandonas, B. G. Ernst, A. Vazquez-Mayagoitia, R. A. DiStasio, and A. Tkatchenko. “QM7-X, a Comprehensive Dataset of Quantum-Mechanical Properties Spanning the Chemical Space of Small Organic Molecules,” *Scientific Data* (February 2021), Springer Nature. doi: 10.1038/s41597-021-00812-2

Seidu, A., M. Dvorak, P. Rinke, and J. Li. “Atomic and Electronic Structure of Cesium Lead Triiodide Surfaces,” *The Journal of Chemical Physics* (February 2021), AIP. doi: 10.1063/5.0035448

Govoni, M., J. Whitmer, J. de Pablo, F. Gygi, and G. Galli. “Code Interoperability Extends the Scope of Quantum Simulations,” *NPJ Computational Materials* (February 2021), Springer Nature. doi: 10.1038/s41524-021-00501-z

Quah, T., and C. O. Iloeje. “Liquid–Liquid Extraction Thermodynamic Parameter Estimator (LLEPE) for Multicomponent Separation Systems,” *Materials Processing Fundamentals* (February 2021), Springer Nature. doi: 10.1007/978-3-030-65253-1_9

Hong, S., S. Tiwari, A. Krishnamoorthy, K. Nomura, C. Sheng, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta. “Sulfurization of MoO3 in the Chemical Vapor Deposition Synthesis of MoS2 Enhanced by an H2S/H2 Mixture,” *The Journal of Physical Chemistry Letters* (February 2021), ACS. doi: 10.1021/acs.jpclett.0c03280

Chan, W. H. R., P. L. Johnson, P. Moin, and J. Urzay. “The Turbulent Bubble Break-up Cascade. Part 2. Numerical Simulations of Breaking Waves,” *Journal of Fluid Mechanics* (February 2021), Cambridge University Press. doi: 10.1017/jfm.2020.1084

New, J. R., B. Bass, M. Adams, and A. Berres. “Model America – Clark County (Vegas) Extract from ORNL’s AutoBEM,” *Zenodo* (February 2021), OpenAIRE. doi: 10.5281/zenodo.4552901

Hu, Z., D. Roten, K. B. Olsen, and S. M. Day. “Modeling of Empirical Transfer Functions with 3D Velocity Structure,” *Bulletin of the Seismological Society of America* (February 2021), GeoScience World. doi: 10.1785/0120200214

Chan, W. H. R., P. L. Johnson, and P. Moin. “The Turbulent Bubble Break-up Cascade. Part 1. Theoretical Developments,” *Journal of Fluid Mechanics* (February 2021), Cambridge University Press. doi: 10.1017/jfm.2020.1083

Zhdankin, V., D. A. Uzdensky, and M. W. Kunz. “Production and Persistence of Extreme Two-Temperature Plasmas in Radiative Relativistic Turbulence,” *The Astrophysical Journal* (February 2021). doi: 10.3847/1538-4357/abcf31

Shin, H., J. T. Krogel, K. Gasperich, P. R. C. Kent, A. Benali, and O. Heinonen. “Optimized Structure and Electronic Band Gap of Monolayer GeSe from Quantum Monte Carlo Methods,” *Physical Review Materials* (February 2021), APS. doi: 10.1103/PhysRevMaterials.5.024002

Saini, N., and I. A. Bolotnov. “Two-Phase Turbulence Statistics from High Fidelity Dispersed Droplet Flow Simulations in a Pressurized Water Reactor (PWR) Sub-Channel with Mixing Vanes,” *Fluids* (February 2021), MDPI. doi: 10.3390/fluids6020072

Vorabbi, M., M. Gennari, P. Finelli, C. Giusti, P. Navrátil, and R. Machleidt. “Impact of Three-Body Forces on Elastic Nucleon–Nucleus Scattering Observables,” *Physical Review C* (February 2021), APS. doi: 10.1103/PhysRevC.103.024604

Yang, L., S. C. Tiwari, S. S. Jo, S. Hong, A. Mishra, A. Krishnamoorthy, R. K. Kalia, A. Nakano, R. Jaramillo, and P. Vashishta. "Unveiling Oxidation Mechanism of Bulk ZrS2," *MRS Advances* (February 2021), Springer Nature. doi: 10.1557/s43580-021-00007-2

Zhou, R., and Y. Kanai. "Dynamical Transition Orbitals: A Particle–hole Description in Real-Time TDDFT Dynamics," *Journal of Chemical Physics* (February 2021), AIP Publishing. doi: 10.1063/5.0035435

Zhao, T., M. Hall, H. Johansen, and S. Williams. "Improving Communication by Optimizing On-Node Data Movement with Data Layout," *PPoPP '21: Proceedings of the 26th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming* (February 2021), ACM Digital Library. doi: 10.1145/3437801.3441598

March

Kowalski, K., R. Bair, N. P. Bauman, J. S. Boschen, E. J. Bylaska, J. Daily, W. A. de Jong, T. Dunning Jr., N. Govind, R. J. Harrison, M. Keceli, K. Keipert, S. Krishnamoorthy, S. Kumar, E. Mutlu, B. Palmer, A. Panyala, B. Peng, R. M. Richard, T. P. Straatsma, P. Sushko, E. F. Valeev, M. Valiev, H. J. J. van Dam, J. M. Waldrop, D. B. Williams-Young, C. Yang, M. Zalewski, and T. L. Windus. "From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape," *Chemical Reviews* (March 2021), ACS Publications. doi: 10.1021/acs.chemrev.0c00998

Wan, S., R. C. Sinclair, and P. V. Coveney. "Uncertainty Quantification in Classical Molecular Dynamics," *Philosophical Transactions of the Royal Society A* (March 2021), The Royal Society. doi: 10.1098/rsta.2020.0082

Ho, P. J., C. Knight, and L. Young. "Fluorescence Intensity Correlation Imaging with High Spatial Resolution and Elemental Contrast Using Intense X-ray Pulses," *Structural Dynamics* (March 2021), AIP Publishing. doi: 10.1063/4.0000105

Caldwell, P. M., C. R. Terai, B. R. Hillman, N. D. Keen, P. A. Bogenschutz, W. Lin, H. Beydoun, M. A. Taylor, L. Bertagna, A. Bradley, T. C. Clevenger, A. S. Donahue, C. Eldred, J. G. Foucar, J.-C. Golaz, O. Guba, R. L. Jacob, J. Johnson, J. Krishna, W. Liu, K. G. Pressel, A. G. Salinger, B. Singh, A. Steyer, P. Ullrich, D. Wu, X. Yuan, J. Shpund, H.-Y. Ma, and C. S. Zender. "Convection-Permitting Simulations with the E3SM Global Atmosphere Model," *Journal of Advances in Modeling Earth System* (March 2021), 2021 American Geophysical Union. doi: 10.1002/essoar.10506530.1

Emani, M., V. Vishwanath, C. Adams, M. E. Papka, R. Stevens, L. Florescu, S. Jairath, W. Liu, T. Nama, and A. Sujeeth. "Accelerating Scientific Applications with SambaNova Reconfigurable Dataflow Architecture," *Computing in Science & Engineering* (March 2021), IEEE. doi: 10.1109/MCSE.2021.3057203

Mulligan, V. K., S. Workman, T. Sun, S. Rettie, X. Li, L. J. Worrall, T. W. Craven, D. T. King, P. Hosseinzadeh, A. M. Watkins, P. D. Renfrew, S. Guffy, J. W. Labonte, R. Moretti, R. Bonneau, N. C. J. Strynadka, and D. Baker. "Computationally Designed Peptide Macrocycle Inhibitors of New Delhi Metallo-β-Lactamase 1," *PNAS – Proceedings of the National Academy of Sciences of the United States of America* (March 2021), National Academy of Science. doi: 10.1073/pnas.2012800118

Deng, G.-H., Y. Qian, X. Li, T. Zhang, W. Jiang, A. R. Harutyunyan, G. Chen, H. Chen, and Y. Rao. "Singlet Fission Driven by Anisotropic Vibronic Coupling in Single-Crystalline Pentacene," *The Journal of Physical Chemistry Letters* (March 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c00397

Jeindl, A., J. Domke, L. Hormann, F. Sojka, R. Forker, T. Fritz, and O. T. Hofmann. "Nonintuitive Surface Self-Assembly of Functionalized Molecules on Ag(111)," *ACS Nano* (March 2021), ACS Publications. doi: 10.1021/acsnano.0c10065

Ayral, T., F.-M. Le Regent, Z. Saleem, Y. Alexeev, and M. Suchara. "Quantum Divide and Compute: Exploring the Effect of Different Noise Sources," *SN Computer Science* (March 2021), Springer Nature. doi: 10.1007/s42979-021-00508-9

Raghavan, K., P. Balaprakash, A. Lovato, N. Rocco, and S. M. Wild. "Machine-Learning-Based Inversion of Nuclear Responses," *Physical Review C* (March 2021), APS. doi: 10.1103/PhysRevC.103.035502

Barrow, J. L., S. Gardiner, S. Pastore, M. Betancourt, and J. Carlson. "Quasielastic Electromagnetic Scattering Cross Sections and World Data Comparisons in the GENIE Monte Carlo Event Generator," *Physical Review D* (March 2021), APS. doi: 10.1103/PhysRevD.103.052001

Maulik, R., B. Lusch, and P. Balaprakash. "Reduced-Order Modeling of Advection-Dominated Systems with Recurrent Neural Networks and Convolutional Autoencoders," *Physics of Fluids* (March 2021), AIP Publishing. doi: 10.1063/5.0039986

Zimmer, M. D., and I. A. Bolotnov. "Evaluation of Length Scales and Meshing Requirements for Resolving Two-Phase Flow Regime Transitions Using the Level Set Method," *Journal of Fluids Engineering* (March 2021), ASME. doi: 10.1115/1.4049934

Akkineni, S., C. Zhu, J. Chen, M. Song, S. Hoff, J. Bonde, J. Tao, H. Heinz, S. Habelitz, and J. De Yoreo. "Amyloid-like Amelogenin Nanoribbons Template Mineralization via a Low Energy Interface of Ion Binding Sites," *Research Square* (March 2021), Research Square, LLC. doi: 10.21203/rs.3.rs-265667/v1

McCracken, C., P. Navrátil, A. McCoy, S. Quaglioni, and G. Hupin. "Microscopic Investigation of the 8Li(n, γ)9 Li Reaction," *Physical Review C* (March 2021), APS. doi: 10.1103/PhysRevC.103.035801

Dong, S. S., M. Govoni, and G. Galli. "Machine Learning Dielectric Screening for the Simulation of Excited State Properties of Molecules and Materials," *Chemical Science* (March 2021), Royal Society of Chemistry. doi: 10.1039/D1SC00503K

April

Pawar, S., and R. Maulik. "Distributed Deep Reinforcement Learning for Simulation Control," *Machine Learning: Science and Technology* (April 2021), IOP Science. doi: 10.1088/2632-2153/abdaf8

New, J. R., B. Bass, M. Adams, A. Berres, and X. Luo. "Los Angeles County Archetypes in Weather Research and Forecasting (WRF) Region from ORNL's AutoBEM," *Zenodo* (April 2021), Zenodo. doi: 10.5281/zenodo.4726136

Islam, T., M. S. Lahijani, A. Srinivasan, S. Namilae, A. Mubayi, and M. Scotch. "From Bad to Worse: Airline Boarding Changes in Response to COVID-19," *Royal Society Open Science* (April 2021), The Royal Society. doi: 10.1098/rsos.201019

Yachnin, B. J., V. K. Mulligan, S. D. Khare, and C. Bailey-Kellogg. "MHCEpitopeEnergy, a Flexible Rosetta-Based Biotherapeutic Deimmunization Platform," *Journal of Chemical Information and Modeling* (April 2021), ACS Publications. doi: 10.1021/acs.jcim.1c00056

Qian, Y., T. Zhang, J. Han, A. R. Harutyunyan, G. Chen, Y. Rao, and H. Chen. "Symmetry-Breaking Enhanced Herzberg-Teller Effect with Brominated Polyacenes," *The Journal of Physical Chemistry A* (April 2021), ACS Publications. doi: 10.1021/acs.jpca.1c01293

Zambre, R., D. Sahasrabudhe, H. Zhou, M. Berzins, and A. Chandramowlish. "Logically Parallel Communication for Fast MPI+Threads Applications," *IEEE Transactions on Parallel and Distributed Systems* (April 2021), IEEE. doi: 10.1109/TPDS.2021.3075157

Boyda, D., G. Kanwar, S. Racanire, D. J. Rezende, M. S. Albergo, K. Cranmer, D. C. Hackett, P. E. Shanahan. "Sampling Using SU (N) Gauge Equivariant Flows," *Physical Review D* (April 2021), APS. doi: 10.1103/PhysRevD.103.074504

Zhou, M., H. A. Doan, L. A. Curtiss, and R. S. Assary. “Identification of Active Metal Carbide and Nitride Catalytic Facets for Hydrodeoxygenation Reactions,” *The Journal of Physical Chemistry C* (April 2021), ACS Publications. doi: 10.1021/acs.jpcc.1c02387

Comeau, D., X. Asay-Davis, C. Begeman, M. Hoffman, W. Lin, M. Petersen, S. Price, A. Roberts, L. Van Roekel, M. Veneziani, and J. Wolfe. “Ice-Shelf Basal Melt Rates in the Energy Exascale Earth System Model (E3SM),” *EGU General Assembly 2021* (April 2021), Copernicus Meetings. doi: 10.5194/egusphere-egu21-13457

Sivaraman, G., L. Gallington, A. N. Krishnamoorthy, M. Stan, G. Csányi, A. Vázquez-Mayagoitia, C. J. Benmore. “Experimentally Driven Automated Machine-Learned Interatomic Potential for a Refractory Oxide,” *Physical Review Letters* (April 2021), APS. doi: 10.1103/physrevlett.126.156002

Perez, J. C., B. D. G. Chandran, K. G. Klein, and M. M. Martinovic. “How Alfven Waves Energize the Solar Wind: Heat versus Work,” *Journal of Plasma Physics* (April 2021), Cambridge University Press. doi: 10.1017/S0022377821000167

Jara-Almonte, J., N. A. Murphy, and H. Ji. “Multi-Fluid and Kinetic Models of Partially Ionized Magnetic Reconnection,” *Physics of Plasma* (April 2021), AIP Publishing. doi: 10.1063/5.0039860

Ruiz, J., K. Misa, A. Seshappan, M. Keceli, and O. Sode. “Exploring the Anharmonic Vibrational Structure of Carbon Dioxide Trimers,” *The Journal of Chemical Physics* (April 2021), AIP Publishing. doi: 10.1063/5.0039793

Mondal, S., R. Torelli, B. Lusch, P. J. Milan, G. M. Magnotti, “Accelerating the Generation of Static Coupling Injection Maps Using a Data-Driven Emulator,” *SAE WCX Digital Summit* (April 2021), SAE International. doi: 10.4271/2021-01-0550

Romano, P. K., S. P. Hamilton, R. O. Rahaman, A. Novak, E. Merzari, S. M. Harper, and P. C. Shriwise. “Design of a Code-Agnostic Driver Application for High-Fidelity Coupled Neutronics and Thermal-Hydraulic Simulations,” *Monte Carlo* (April 2021), ADS. doi: 10.1051/epjconf/202124706053

May

Javadi, A., T. Jamil, E. Abouzari-Lotf, M. D. Soucek, and H. Heinz. “Working Mechanisms and Design Principles of Comb-like Polycarboxylate Ether Superplasticizers in Cement Hydration: Quantitative Insights for a Series of Well-Defined Copolymers,” *ACS Sustainable Chemistry & Engineering* (May 2021), ACS Publications. doi: 10.1021/acssuschemeng.0c08566

Larsson, J., “Simple Inflow Sponge for Faster Turbulent Boundary-Layer Development,” *AIAAJ Aeronautics/Astronautics* (May, 2021), American Institute of Aeronautics and Astronautics, Inc., doi: 10.2514/1.J060721

Gligorijević, V., P. D. Renfrew, T. Kosciolek, J. Koehler Leman, D. Berenberg, T. Vatanen, C. Chandler, B. C. Taylor, I. M. Fisk, H. Vlamakis, R. J. Xavier, R, Knight, K. Cho, and R. Bonneau. “Structure-Based Protein Function Prediction Using Graph Convolutional Networks,” *Nature Communications* (May 2021), Springer Nature. doi: 10.1038/s41467-021-23303-9

Saidi, W. A., W. Shadid, and G. Veser. “Optimization of High-Entropy Alloy Catalyst for Ammonia Decomposition and Ammonia Synthesis,” *The Journal of Physical Chemistry Letters* (May 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c01242

Peterson, J. R., S. Glenzer, and F. Fiuza. “Magnetic Field Amplification by a Nonlinear Electron Streaming Instability,” *Physical Review Letters* (May 2021), APS. doi: 10.1103/physrevlett.126.215101

Krishnamoorthy, A., K. Nomura, N. Baradwaj, K. Shimamura, P. Rajak, A. Mishra, S. Fukushima, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. “Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics,” *Physical Review Letters* (May 2021), APS. doi: 10.1103/PhysRevLett.126.216403

Wilamowski, M., D. A. Sherrell, G. Minasov, Y. Kim, L. Shuvalova, A. Lavens, R. Chard, N. Maltseva, R. Jedrzejczak, M. Rosas-Lemus, N. Saint, I. T. Foster, K. Michalska, K. J. F. Satchell, and A. Joachimiak. “2′-O Methylation of RNA Cap in SARS-CoV-2 Captured by Serial Crystallography,” *PNAS – Proceedings of the National Academy of Sciences of the United States of America* (May 2021), National Academy of Science. doi: 10.1073/pnas.2100170118

Valassi, A., E. Yazgan, J. McFayden, S. Amoroso, J. Bendavid, A. Buckley, M. Cacciari, T. Childers, V. Ciulli, R. Frederix, S. Frixione, F. Giuli, A. Grohsjean, C. Gütschow, S. Höche, W. Hopkins, P. Ilten, D. Konstantinov, F. Krauss, Q. Li, L. Lönnblad, F. Maltoni, M. Mangano, Z. Marshall, O. Mattelaer, J. F. Menendez, S. Mrenna, S. Muralidharan, T. Neumann, S. Plätzer, S. Prestel, S. Roiser, M. Schönherr, H. Schulz, M. Schulz, E. Sexton-Kennedy, F. Siegert, A. Siódmok, and G. A. Stewart. “Challenges in Monte Carlo Event Generator Software for High-Luminosity LHC,” *Computing and Software for Big Science* (May 2021), Springer. doi: 10.1007/s41781-021-00055-1

Annaberdiyev, A., G. Wang, C. A. Melton, M. C. Bennett, and L. Mitas. “Cohesion and Excitations of Diamond-Structure Silicon by Quantum Monte Carlo: Benchmarks and Control of Systematic Biases,” *Physical Review B* (May 2021), APS. doi: 10.1103/PhysRevB.103.205206

Shaffer, T., Z. Li, B. Tovar, Y. Babuji, T. J. Dasso, Z. Surma, K. Chard, I. Foster, and D. Thain. “Lightweight Function Monitors for Fine-Grained Management in Large Scale Python Applications,” *2021 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (May 2021), IEEE. doi: 10.1109/IPDPS49936.2021.00088

Ramesh, S., A. D. Malony, P. Carns, R. B. Ross, M. Dorier, J. Soumagne, and S. Snyder, “SYMBIOSYS: A Methodology for Performance Analysis of Composable HPC Data Services,” *2021 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (May 2021), IEEE. doi: 10.1109/IPDPS49936.2021.00013

Bao, J.-K., D. E. Bugaris, H. Zheng, D. Y. Chung, and M. G. Kanatzidis. “A Noncentrosymmetric Polymorph of LuRuGe,” *Inorganic Chemistry* (May 2021), ACS Publications. doi: 10.1021/acs.inorgchem.1c00320

Fan, Y., Z. Lan, T. Childers, P. Rich, W. Allcock, and M. E. Papka. “Deep Reinforcement Agent for Scheduling in HPC,” *2021 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (May 2021), IEEE Xplore. doi: 10.1109/IPDPS49936.2021.00090

Partin, A., T. Brettin, Y. A. Evrard, Y. Zhu, H. Yoo, F. Xia, S. Jiang, A. Clyde, M. Shukla, M. Fonstein, J. H. Doroshow, and R. L. Stevens. “Learning Curves for Drug Response Prediction in Cancer Cell Lines,” *PubMed* (May 2021), National Library of Medicine. doi: 10.1186/s12859-021-04163-y

Devarajan, H., H. Zheng, A. Kougkas, X.-H. Sun, and V. Vishwanath. “DLIO: A Data-Centric Benchmark for Scientific Deep Learning Applications,” *2021 IEEE/ACM 21st International Symposium on Cluster, Cloud and Internet Computing (CCGrid)* (May 2021), IEEE. doi: 10.1109/CCGrid51090.2021.00018

Li, M., M. T. Curnan, M. A. Gresh-Sill, S. D. House, W. A. Saidi, and J. C. Yang. “Unusual Layer-by-Layer Growth of Epitaxial Oxide Islands during Cu Oxidation,” *Nature Communications* (May 2021), Nature Portfolio. doi: 10.1038/s41467-021-23043-w

Yang, C. J., A. Ekstrom, C. Forssen, and G. Hagen. “Power Counting in Chiral Effective Field Theory and Nuclear Binding,” *Physical Review C* (May 2021), APS. doi: 10.1103/PhysRevC.103.054304

Novario, S., P. Gysbers, J. Engel, G. Hagen, G. R. Jansen, T. D. Morris, P. Navrátil, T. Papenbrock, and S. Quaglioni. “Coupled-Cluster Calculations of Neutrinoless Double-β Decay in 48 Ca,” *Physical Review Letters* (May 2021), APS. doi: 10.1103/PhysRevLett.126.182502

Balin, R., and K. E. Jansen. “Direct Numerical Simulation of a Turbulent Boundary Layer over a Bump with Strong Pressure Gradients,” *Journal of Fluid Mechanics* (May 2021), Cambridge University Press. doi: 10.1017/jfm.2021.312

Keskinen, K., G. Giannakopoulos, M. Bolla, J. Koch, Y. M. Wright, C. Frouzakis, K. Boulouchos, M. Schmidt, B. Böhm, and A. Dreizler. "Novel Insight into Engine Near-Wall Flows and Wall Heat Transfer Using Direct Numerical Simulations and High-Fidelity Experiments," *Internationales Stuttgarter Symposium* (May 2021), Springer Vieweg, Wiesbaden. doi: 10.1007/978-3-658-33521-2_26

Maris, P., E. Epelbaum, R. J. Furnstahl, J. Golak, K. Hebeler, T. Huther, H. Kamada, H. Krebs, Ulf-G. Meiner, J. A. Melendez, A. Nogga, P. Reinert, R. Roth, R. Skibinski, V. Soloviov, K. Topolnicki, J. P. Vary, Yu. Volkotrub, H. Witala, and T. Wolfgruber (LENPIC Collaboration). "Light Nuclei with Semilocal Momentum-Space Regularized Chiral Interactions up to Third Order," *Physical Review C* (May 2021), APS. doi: 10.1103/PhysRevC.103.054001

Srinivasan, S., R. Batra, H. Chan, G. Kamath, M. J. Cherukara, and S. K. R. S. Sankaranarayanan. "Artificial Intelligence-Guided De Novo Molecular Design Targeting COVID-19," *ACS Omega* (May 2021), ACS Publications. doi: 10.1021/acsomega.1c00477

Chan, W. H. R., M. S. Dodd, P. L. Johnson, and P. Moin. "Identifying and Tracking Bubbles and Drops in Simulations: A Toolbox for Obtaining Sizes, Lineages, and Breakup and Coalescence Statistics," *Journal of Computational Physics* (May 2021), Elsevier. doi: 10.1016/j.jcp.2021.110156

Schiavilla, R., L. Girlanda, A. Gnech, A. Kievesky, A. Lovato, L. E. Marcucci, M. Piarulli, and M. Viviani. "Two- and Three-Nucleon Contact Interactions and Ground-State Energies of Light- and Medium-Mass Nuclei," *Physical Review C* (May 2021), ADS. doi: 10.1103/physrevc.103.054003

June

Ward, L., N. Dandu, B. Blaiszik, B. Narayanan, R. S. Assary, P. C. Redfern, I. Foster, and L. A. Curtiss. "Graph-Based Approaches for Predicting Solvation Energy in Multiple Solvents: Open Datasets and Machine Learning Models," *The Journal of Physical Chemistry A* (June 2021), ACS Publications. doi: 10.1021/acs.jpca.1c01960

Rasquin, M., K. Hillewaert, A. Colombo, F. Bassi, F. Massa, K. Puri, A. S. Iyer, Y. Abe, F. D. Witherden, B. C. Vermeire, and P. E. Vincent. "Computational Campaign on the MTU T161 Cascade," *TILDA: Towards Industrial LES/DNS in Aeronautics* (June 2021), Springer International Publishing. doi: 10.1007/978-3-030-62048-6_18

Xie, B., Z. Tan, P. Carns, J. Chase, K. Harms, J. Lofstead, S. Oral, S. S. Vazhkudai, and F. Wang. "Interpreting Write Performance of Supercomputer I/O Systems with Regression Models," *2021 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (June 2021), IEEE. doi: 10.1109/IPDPS49936.2021.00064

Nagakura, H., A. Burrows, and D. Vartanyan. "Supernova Neutrino Signals Based on Long-Term Axisymmetric Simulations," *Monthly Notices of the Royal Astronomical Society* (June 2021), Oxford Academic. doi: 10.1093/mnras/stab1785

Di Renzo, M., N. Oberoi, J. Larsson, and S. Pirozzoli. "Crossflow Effects on Shock Wave/Turbulent Boundary Layer Interactions," *Theoretical and Computational Fluid Dynamics* (June 2021), SpringerLink. doi: 10.1007/s00162-021-00574-y

Pan, K.-C., M. Liebendörfer, S. M. Couch, and F.-K. Thielemann. "Stellar Mass Black Hole Formation and Multimessenger Signals from Three-dimensional Rotating Core-Collapse Supernova Simulations," *The Astrophysical Journal* (June 2021), IOP Science. doi: 10.3847/1538-4357/abfb05

Rajak, P., N. Baradwaj, K. Nomura, A. Krishnamoorthy, J. P. Rino, K. Shimamura, S. Fukushima, F. Shimojo, R. Kalia, A. Nakano, and P. Vashishta. "Neural Network Quantum Molecular Dynamics, Intermediate Range Order in GeSe2, and Neutron Scattering Experiments," *The Journal of Physical Chemistry Letters* (June 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c01272

Demiroglu, I., Y. Karaaslan, T. Kocabas, M. Keceli, A. Vazquez-Mayagoitia, and C. Sevik. "Computation of the Thermal Expansion Coefficient of Graphene with Gaussian Approximation Potentials," *The Journal of Physical Chemistry C* (June 2021), ACS Publications. doi: 10.1021/acs.jpcc.1c01888

Skluzacek, T. J., R. Wong, Z. Li, R. Chard, K. Chard, and I. Foster. "A Serverless Framework for Distributed Bulk Metadata Extraction," *HPDC '21: Proceedings of the 30th International Symposium on High-Performance Parallel and Distributed Computing* (June 2021), ACM Digital Library. doi: 10.1145/3431379.3460636

Rajak, P., A. Aditya, S. Fukushima, R. K. Kalia, T. Linker, K. Liu, Y. Luo, A. Nakano, K. Nomura, K. Shimamura, F. Shimojo, and P. Vashishta. "Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics," *2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)* (June 2021), IEEE. doi: 10.1109/IPDPSW52791.2021.00145

Pajkos, M. A., M. L. Warren, S. M. Couch, E. P. O'Connor, and K.-C. Pan. "Determining the Structure of Rotating Massive Stellar Cores with Gravitational Waves," *The Astrophysical Journal* (June 2021), IOP Science. doi: 10.3847/1538-4357/abfb65

Brown, K. A., N. McGlohon, S. Chunduri, E. Borch, R. B. Ross, C. D. Carothers, and K. Harms. "A Tunable Implementation of Quality-of-Service Classes for HPC Networks," *ISC High Performance 2021: International Conference on High Performance Computing* (June 2021), Springer Nature. doi: 10.1007/978-3-030-78713-4_8

Vazquez, H., A. Kononov, A. Kyritsakis, N. Medvedev, A. Schleife, and F. Djurabekova. "Electron Cascades and Secondary Electron Emission in Graphene under Energetic Ion Irradiation," *Physical Review B* (June 2021), APS. doi: 10.1103/PhysRevB.103.224306

Zahariev, F., and M. S. Gordon. "Combined Quantum Monte Carlo — Effective Fragment Molecular Orbital Method: Fragmentation across Covalent Bonds," *Physical Chemistry Chemistry Physics* (June 2021), Royal Society of Chemistry. doi: 10.1039/D0CP06528E

Nemani, S., K., B. Zhang, B. C. Wyatt, Z. D. Hood, S. Manna, R. Khaledialidusti, W. Hong, M. G. Sternberg, S. K. R. S. Sankaranarayanan, B. Anasori. "High-Entropy 2D Carbide MXenes: TiVNbMoC3 and TiVCrMoC3," *ASC Nano* (June 2021), ACS Publications. doi: 10.1021/acsnano.1c02775

Hall, C. L., I. Andrusenko, J. Potticary, S. Gao, X. Liu, W. Schmidt, N. Marom, E. Mugnaioli, M. Gemmi, and S. R. Hall. "3D Electron Diffraction Structure Determination of Terrylene, a Promising Candidate for Intermolecular Singlet Fission," *ChemPhysChem* (June 2021), Chemistry Europe. doi: 10.1002/cphc.202100320

Ma, P.-X., X. Feng, M. Gorchtein, L.-C. Jin, and C.-Y. Seng. "Lattice QCD Calculation of the Electroweak Box Diagrams for the Kaon Semileptonic Decays," *Physical Review D* (June 2021), APS. doi: 10.1103/PhysRevD.103.114503

Sastry, V. K., R. Maulik, V. Rao, B. Lusch, S. A. Renganathan, and R. Kotamarthi. "Data-Driven Deep Learning Emulators for Geophysical Forecasting," *International Conference on Computational Science ICCS 2021: Computational Science* (June 2021), SpringerLink. doi: 10.1007/978-3-030-77977-1_35

Hosseinzadeh, P., P. R. Watson, T. W. Craven, X. Li, S. Rettie, F. Pardo-Avila, A. K. Bera, V. K. Mulligan, P. Lu, A. S. Ford, B. D. Weitzner, L. J. Stewart, A. P. Moyer, M. Di Piazza, J. G. Whalen, P.Greisen, Jr., D. W. Christianson, and D. Baker. "Anchor Extension: A Structure-Guided Approach to Design Cyclic Peptides Targeting Enzyme Active Sites," *Nature Communications* (June 2021), Springer Nature. doi: 10.1038/s41467-021-23609-8

Evans, D. J., R. A. Yovanno, S. Rahman, D. W. Cao, M. Q. Beckett, M. H. Patel, A. F. Bandak, and A. Y. Lau. "Finding Druggable Sites in Proteins Using TACTICS," *Journal of Chemical Information and Modeling* (June 2021), ACS Publications. doi: 10.1021/acs.jcim.1c00204

Leong, T., C. Voleti, and Z. Peng. “Coarse-Grained Modeling of Coronavirus Spike Proteins and ACE2 Receptors,” *Frontiers in Physics* (June 2021), Frontier Media. doi: 10.3389/fphy.2021.680983

Chopineau, L., A. Denoeud, A. Leblanc, E. Porat, P. Martin, H. Vincenti, and F. Qu√©r√©. “Spatio-Temporal Characterization of Attosecond Pulses from Plasma Mirrors,” *Nature Physics* (June 2021), Nature Physics. doi: 10.1038/s41567-021-01253-9

Muniz, M. C., T. E. Gartner III, M. Riera, C. Knight, S. Yue, F. Paesani, and A. Z. Panagiotopoulos. “Vapor–Liquid Equilibrium of Water with the MB-pol Many-Body Potential,” *The Journal of Chemical Physics* (June 2021), AIP Publishing. doi: 10.1063/5.0050068

July

Schwartz, J., C. Harris, J. Pietryga, H. Zheng, P. Kumar, A. Visheratina, N. Kotov, Y. Jiang, M. Hanwell, and R. Hovden. “Real-Time 3D Analysis during Tomographic Experiments on tomviz,” *Microscopy and Microanalysis* (July 2021), Cambridge University Press. doi: 10.1017/S1431927621009983

Schwartz, J., Y. Jiang, Z. W. Di, T. Ma, H. Zheng, S. Rozeveld, and R. Hovden. “Recovering Chemistry at Atomic Resolution using Multi-Modal Spectroscopy,” *Microscopy and Microanalysis* (July 2021), Cambridge University Press. doi: 10.1017/S1431927621004608

Kurihana, T., E. Moyer, R. Willett, D. Gilton, and I. Foster. “Data-Driven Cloud Clustering via a Rotationally Invariant Autoencoder,” *IEEE Transactions on Geoscience and Remote Sensing* (July 2021), IEEE. doi: 10.1109/TGRS.2021.3098008

Sun, Y. Z. S., R. F. DeJaco, Z. Li, D. Tang, S. Glante, D. S. Sholl, C. M. Colina, R. Q. Snurr, M. Thommes, M. Hartmann, J. I. Siepmann. “Fingerprinting Diverse Nanoporous Materials for Optimal Hydrogen Storage Conditions Using Meta-Learning,” *Science Advances* (July 2021), AAAS. doi: 10.1126/sciadv.abg3983

Andolina, C. M., M. Bon, D. Passerone, and W. A. Saidi. “Robust, Multi-Length-Scale, Machine Learning Potential for Ag–Au Bimetallic Alloys from Clusters to Bulk Materials,” *American Chemical Society* (July 2021), ACS Publications. doi: 10.1021/acs.jpcc.1c04403

Banik, S., T. D. Loeffler, R. Batra, H. Singh, M. J. Cherukara, and S. K. R. S. Sankaranarayanan. “Learning with Delayed Rewards — A Case Study on Inverse Defect Design in 2D Materials,” *American Chemical Society* (July 2021), ACS Publications. doi: 10.1021/acsami.1c07545

Datta, D., and M. S. Gordon. “A Massively Parallel Implementation of the CCSD(T) Method Using the Resolution-of-the-Identity Approximation and a Hybrid Distributed/Shared Memory Parallelization Model,” *Journal of Chemical Theory and Computation* (July 2021), ACS Publications. doi: 10.1021/acs.jctc.1c00389

Jimenez, D., E. Meneses, and V. I. Vargas. “Adaptive Plasma Physics Simulations: Dealing with Load Imbalance using Charm++,” *PEARC ’21: Practice and Experience in Advanced Research Computing* (July 2021), ACM Digital Library. doi: 10.1145/3437359.3465566

Campos-Duarte, L., D. Jimenez, E. Meneses, R. Solano-Piedra, E. Perez, and V. I. Vargas. “Towards Photorealistic Visualizations for Plasma Confinement Simulations,” *PEARC ’21: Practice and Experience in Advanced Research Computing* (July 2021), ACM Digital Library. doi: 10.1145/3437359.3465608

Norman, M. R., D. A. Bader, C. Eldred, W. M. Hannah, B. R. Hillman, C. R. Jones, J. M. Lee, L. R. Leung, I. Lyngaas, K. G. Pressel, S. Sreepathi, M. A. Taylor, and X. Yuan. “Unprecedented Cloud Resolution in a GPU-Enabled Full-Physics Atmospheric Climate Simulation on OLCF’s Summit Supercomputer,” *The International Journal of High Performance Computing Applications* (July 2021), Sage Publications. doi: 10.1177/10943420211027539

Rajak, P., A. Krishnamoorthy, A. Mishra, R. Kalia, A. Nakano, and P. Vashishta. “Autonomous Reinforcement Learning Agent for Chemical Vapor Deposition Synthesis of Quantum Materials,” *NPJ Computational Materials* (July 2021), Springer Nature. doi: 10.1038/s41524-021-00535-3

Wang, S., K. Hou, and H. Heinz. “Accurate and Compatible Force Fields for Molecular Oxygen, Nitrogen, and Hydrogen to Simulate Gases, Electrolytes, and Heterogeneous Interfaces,” *Journal of Chemical Theory and Computation* (July 2021), ACS Publications. doi: 10.1021/acs.jctc.0c01132

Rajak, P., B. Wang, K. Nomura, Y. Luo, A. Nakano, R. Kalia, and P. Vashishta. “Autonomous Reinforcement Learning Agent for Stretchable Kirigami Design of 2D Materials,” *NPJ Computational Materials* (July 2021), Springer Nature. doi: 10.1038/s41524-021-00572-y

Yao, Y., and Y. Kanai. “Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network,” *The Journal of Physical Chemistry Letters* (July 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c01566

Lykov, D., and Y. Alexeev. “Importance of Diagonal Gates in Tensor Network Simulations,” *2021 IEEE Computer Society Annual Symposium on VLSI* (July 2021), IEEE. doi: 10.1109/isvlsi51109.2021.00088

Lee, H., A. Merzky, L. Tan, M. Titov, M. Turilli, D. Alfe, A. Bhati, A. Brace, A. Clyde, P. Coveney, H. Ma, A. Ramanathan, R. Stevens, A. Trifan, H. V. Dam, S. Wan, S. Wilkinson, and S. Jha. “Scalable HPC & AI infrastructure for COVID-19 Therapeutics,” *PASC ’21: Proceedings of the Platform for Advanced Scientific Computing Conference* (July 2021), ACM Digital Library. doi: 10.1145/3468267.3470573

Huerta, E. A., A. Khan, X. Huang, M. Tian, M. Levental, R. Chard, W. Wei, M. Heflin, D. S. Katz, V. Kindratenko, D. Mu, B. Blaiszik, and I. Foster. “Accelerated, Scalable and Reproducible AI-Driven Gravitational Wave Detection,” *Nature Astronomy* (July 2021), Springer Nature. doi: 10.1038/s41550-021-01405-0

McCaskey, A., T. Nguyen, A. Santana, D. Claudino, T. Kharazi, and H. Finkel. “Extending C++ for Heterogeneous Quantum-Classical Computing,” *ACM Transactions on Quantum Computing* (July 2021), Association for Computing Machinery (ACM). doi: 10.1145/3462670

Mniszewski, S. M., J. Belak, J.-L. Fattebert, C. F. A. Negre, S. R. Slattery, A. A. Adedoyin, R. F. Bird, C. Chang, G. C., S. Ethier, S. Fogerty, S. Habib, C. Junghans, D. Lebrun-Grandi, J. Mohd-Yusof, S. G. Moore, D. Osei-Kuffuor, S. J. Plimpton, A. Pope, S. T. Reeve, L. Ricketson, A. Scheinberg, A. Y. Sharma, and M. E. Wall. “Enabling Particle Applications for Exascale Computing Platforms,” *International Journal of High Performance Computing Applications* (July 2021), Sage Publications. doi: 10.1177/10943420211022829

August

Hong, Z., G. Pauloski, L. Ward, K. Chard, B. Blaiszik, and I. Foster. “Models and Processes to Extract Drug-like Molecules From Natural Language Text,” *Frontiers in Molecular Biosciences* (August 2021), Frontier Media. doi: 10.3389/fmolb.2021.636077

Brace, A., M. Salim, V. Subbiah, H. Ma, M. Emani, A. Trifa, A. R. Clyde, C. Adams, T. Uram, H. Yoo, A. Hock, J. Liu, V. Vishwanath, and A. Ramanathan. “Stream-AI-MD: Streaming AI-Driven Adaptive Molecular Simulations for Heterogeneous Computing Platforms,” *PASC ’21: Proceedings of the Platform for Advanced Scientific Computing Conference* (August 2021), ACM Digital Library. doi: 10.1145/3468267.3470578

Fu, L., S. Bose, and P. Moin. “Prediction of Aerothermal Characteristics of a Generic Hypersonic Inlet Flow,” *Theoretical and Computational Fluid Dynamics* (August 2021), Springer Nature. doi: 10.1007/s00162-021-00587-7

Saini, N., and I. A. Bolotnov. “Detailed Analysis of the Effects of Spacer Grid and Mixing Vanes on Turbulence in a PWR Subchannel under DFFB Conditions Based on DNS Data,” *Nuclear Technology* (August 2021), Taylor & Francis Online. doi: 10.1080/00295450.2021.1974279

Andolina, C. M., J. G. Wright, N. Das, and W. A. Saidi. “Improved Al-Mg Alloy Surface Segregation Predictions with a Machine Learning Atomistic Potential,” *Physical Review Materials* (August 2021), APS. doi: 10.1103/physrevmaterials.5.083804

Jin, Y., M. Govoni, G. Wolfowicz, S. E. Sullivan, F. J. Heremans, D. D. Awschalom, and G. Galli. “Photoluminescence Spectra of Point Defects in Semiconductors: Validation of First-Principles Calculations,” *Physical Review Materials* (August 2021), APS. doi: 10.1103/PhysRevMaterials.5.084603

Charity, R. J., T. B. Webb, J. M. Elson, D. E. M. Hoff, C. D. Pruitt, L. G. Sobotka, P. Navrátil, G. Hupin, K. Kravvaris, S. Quaglioni, K. W. Brown, G. Cerizza, J. Estee, W. G. Lynch, J. Manfredi, P. Morfouace, C. Santamaria, S. Sweany, M. B. Tsang, T. Tsang, K. Zhu, S. A. Kuvin, D. McNeel, J. Smith, A. H. Wousmaa, and Z. Chajecki. “Using Spin Alignment of Inelastically Excited Nuclei in Fast Beams to Assign Spins: The Spectroscopy of 13 O as a Test Case,” *Physical Review C* (August 2021), APS. doi: 10.1103/PhysRevC.104.024325

Lopez-Gomez, J., and J. Blomer. “Exploring Object Stores for High-Energy Physics Data Storage,” *EPJ Web* (August 2021), EDP Sciences. doi: 10.1051/epjconf/202125102066

Buchmeier, J., A. Bumann, X. Gao, and I. Bermejo-Moreno. “Geometry and Dynamics of Passive Scalar Structures in Compressible Turbulent Mixing,” *Physics of Fluids* (August 2021), AIP Publishing. doi: 10.1063/5.0068010

Merzky, A., M. Turilli, M. Titov, A. Al Saadi, and S. Jha. “Design and Performance Characterization of RADICAL-Pilot on Leadership-Class Platforms,” *IEEE Transactions on Parallel and Distributed Systems* (August 2021), IEEE. doi: 10.1109/TPDS.2021.3105994

Hamzi, B., R. Maulik, and H. Owhadi. “Simple, Low-Cost and Accurate Data-Driven Geophysical Forecasting with Learned Kernels,” *Proceedings of the Royal Society A: Mathematical, Physical, and Engineering Sciences* (August 2021), The Royal Society. doi: 10.1098/rspa.2021.0326

Wang, Y., and C. Goulet. “Validation of Fault Displacements from Dynamic Rupture Simulations against the Observations from the 1992 Landers Earthquake,” *Bulletin of the Seismological Society of America* (August 2021), GeoScience World. doi: 10.1785/0120210082

Jana, M. K., R. Song, Y. Xie, R. Zhao, P. C. Sercel, V. Blum, and D. B. Mitzi. “Structural Descriptor for Enhanced Spin-Splitting in 2D Hybrid Perovskites,” *Nature Communications* (August 2021), Nature Communications. doi: 10.1038/s41467-021-25149-7

Froese, P., and P. Navrátil. “Ab Initio Calculations of Electric Dipole Moments of Light Nuclei,” *Physical Review C* (August 2021), APS. doi: 10.1103/PhysRevC.104.025502

Sobczyk, J. E., B. Acharya, S. Bacca, and G. Hagen. “Ab Initio Computation of the Longitudinal Response Function in 40 Ca,” *Physical Review Letters* (August 2021), APS. doi: 10.1103/PhysRevLett.127.072501

Saadi, A. A., D. Alfe, Y. Babuji, A. Bhati, B. Blaiszik, T. Brettin, K. Chard, R. Chard, P. Coveney, A. Trifan, A. Brace, A. Clyde, I. Foster, T. Gibbs, S. Jha, K. Keipert, T. Kurth, D. Kranzlmüller, H. Lee, Z. Li, H. Ma, A. Merzky, G. Mathias, A. Partin, J. Yin, A. Ramanathan, A. Shah, A. Stern, R. Stevens, L. Tan, M. Titov, A. Tsaris, M. Turilli, H. V. Dam, S. Wan, and D. Wifling. “IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads,” *ICPP 2021: 50th International Conference on Parallel Processing* (August 2021), ACM Digital Library. doi: 10.1145/3472456.3473524

Bian, X., J. K. Shang, E. G. Blackman, G. W. Collins, and H. Aluie. “Scaling of Turbulent Viscosity and Resistivity: Extracting a Scale-Dependent Turbulent Magnetic Prandtl Number,” *The Astrophysical Journal* (August 2021), The American Astronomical Society. doi: 10.3847/2041-8213/ac0fe5

Lee, D., S. Bogner, B. A. Brown, S. Elhatisari, E. Epelbaum, H. Hergert, M. Hjorth-Jensen, H. Krebs, N. Li, B.-N. Lu, and U.-G. Meißner. “Hidden Spin–Isospin Exchange Symmetry,” *Physical Review Letters* (August 2021), APS. doi: 10.1103/PhysRevLett.127.062501

September

Huerta, E. A., and Z. Zhao. “Advances in Machine and Deep Learning for Modeling and Real-Time Detection of Multi-Messenger Sources,” *Handbook of Gravitational Wave Astronomy* (September 2021), Springer Nature. doi: 10.1007/978-981-15-4702-7_47-1

Caprio, M. A., P. J. Fasano, P. Maris, and A. E. McCoy. “Quadrupole Moments and Proton-Neutron Structure in p -shell Mirror Nuclei,” *Physical Review C* (September 2021), APS. doi: 10.1103/PhysRevC.104.034319

Sun, G., and P. Sautet. “Active Site Fluxional Restructuring as a New Paradigm in Triggering Reaction Activity for Nanocluster Catalysis,” *Accounts of Chemical Research* (September 2021), ACS Publications. doi: 10.1021/acs.accounts.1c00413

Maguire, J. B., D. Grattarola, V. K. Mulligan, E. Klyshko, and H. Melo. “XENet: Using a New Graph Convolution to Accelerate the Timeline for Protein Design on Quantum Computers,” *PLOS Computational Biology* (September 2021), PLOS. doi: 10.1371/journal.pcbi.1009037

Bao, J.-K., H. Zheng, J. Wen, S. Ramakrishnan, H. Zheng, J. S. Jiang, D. Bugaris, G. Cao, D. Y. Chung, S. van Smaalen, and M. G. Kanatzidis. “Superconductivity in Y4RuGe8 with a Vacancy-Ordered CeNiSi2-Type Superstructure,” *Chemistry of Materials* (September 2021), ACS Publications. doi: 10.1021/acs.chemmater.1c02488

Mougeot, M., D. Atanasov, J. Karthein, R. N. Wolf, P. Ascher, K. Blaum, K. Chrysalidis, G. Hagen, J. D. Holt, W. J. Huang, G. R. Jansen, I. Kulikov, Y. A. Litvinov, D. Lunney, V. Manea, T. Miyagi, T. Papenbrock, L. Schweikhard, A. Schwenk, T. Steinsberger, S. R. Stroberg, Z. H. Sun, A. Welker, F. Wienholtz, S. G. Wilkins, and K. Zuber. “Mass Measurements of 99-101 In Challenge Ab Initio Nuclear Theory of the Nuclide 100 Sn,” *Nature Physics* (September 2021), Springer Nature. doi: 10.1038/s41567-021-01326-9

Ahn, J., I. Hong, G. Lee, H. Shin, A. Benali, and Y. Kwon. “Adsorption of a Single Pt Atom on Graphene: Spin Crossing between Physisorbed Triplet and Chemisorbed Singlet States,” *Physical Chemistry Chemistry Physics* (September 2021), Royal Society of Chemistry. doi: 10.1039/D1CP02473F

Shen, S., T. A. Lahde, and D. L. U. G. Meibner. “Wigner SU(4) Symmetry, Clustering, and the Spectrum of 12C,” *The European Physical Journal A* (September 2021), Springer Nature. doi: 10.1140/epja/s10050-021-00586-6

Schmidt, D., R. Maulik, and K. Lyras. “Machine Learning Accelerated Turbulence Modeling of Transient Flashing Jets,” *AIP Physics of Fluids* (September 2021), AIP Publishing. doi: 10.1063/5.0072180

Prayogo, G. I., H. Shin, A. Benali, R. Maezono, and K. Hongo. “Importance of Van der Waals Interactions in Hydrogen Adsorption on a Silicon–Carbide Nanotube Revisited with vdW-DFT and Quantum Monte Carlo,” *ACS Omega* (September 2021), ACS Publications doi: 10.1021/acsomega.1c03318

Mulligan, V. K. “Current Directions in Combining Simulation-Based Macromolecular Modeling Approaches with Deep Learning,” *Expert Opinion on Drug Discovery* (September 2021), Taylor & Francis Online. doi: 10.1080/17460441.2021.1918097

Krishnamoorthy, A., S. C. Tiwari, A. Nakano, R. K. Kalia, and P. Vashishta. "Electric-Field-Induced Crossover of Polarization Reversal Mechanisms in Al1–xScxN Ferroelectrics," *Nanotechnology* (September 2021), IOP Science. doi: 10.1088/1361-6528/ac20fc

Moberg, D. R., A. W. Jasper, and M. J. Davis. "Parsimonious Potential Energy Surface Expansions Using Dictionary Learning with Multipass Greedy Selection," *The Journal of Physical Chemistry Letters* (September 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c02721

Court, C. J., A. Jain, and J. M. Cole. "Inverse Design of Materials That Exhibit the Magnetocaloric Effect by Text-Mining of the Scientific Literature and Generative Deep Learning," *Chemistry of Materials* (September 2021), ACS Publications. doi: 10.1021/acs.chemmater.1c01368

Pillai, N., N. L. Sponsel, K. Stapelmann, and I. A. Bolotnov. "Direct Numerical Simulation of Bubble Formation through a Submerged 'Flute' with Experimental Validation," *Journal of Fluids Engineering* (September 2021), ASME. doi: 10.1115/1.4052051

Poltev, V., V. M. Anisimov, V. Dominguez, A. Ruiz, A. Deriabina, E. Gonzalez, D. Garcia, and F. Rivas. "Understanding the Origin of Structural Diversity of DNA Double Helix," *Computation* (September 2021), MDPI. doi: 10.3390/computation9090098

Ozik, J., J. M. Wozniak, N. Collier, C. M. Macal, and M. Binois. "A Population Data-Driven Workflow for COVID-19 Modeling and Learning," *The International Journal of High Performance Computing Applications* (September 2021), Sage Publications. doi: 10.1177/10943420211035164

Shepard, C., R. Zhou, D. C. Yost, Y. Yao, and Y. Kanai. "Simulating Electronic Excitation and Dynamics with Real-Time Propagation Approach to TDDFT within Plane-Wave Pseudopotential Formulation," *The Journal of Chemical Physics* (September 2021), AIP Publishing. doi: 10.1063/5.0057587

Wong, C., and Y. Kanai. "First Principles Dynamics Study of Excited Hole Relaxation in DNA," *ChemPhysChem* (September 2021), John Wiley & Sons. doi: 10.1002/cphc.202100521

O'Reilly, O., T.-Y. Yeh, K. B. Olsen, Z. Hu, A. Breuer, D. Roten, and C. A. Goulet. "A High-Order Finite-Difference Method on Staggered Curvilinear Grids for Seismic Wave Propagation Applications with Topography," *Bulletin of the Seismological Society of America* (September 2021), GeoScience World. doi: 10.1785/0120210096

Bass, B., J. R. New, E. Ezell, P. Im, E. Garrison, and W. Copeland. "Utility-Scale Building Type Assignment Using Smart Meter Data," *Conference: Building Simulation Conference (BuildSim 2021)* (September 2021), OSTI.

Li, M., D. Liu, X. Chen, Z. Yin, H. Shen, A. Aiello, K. R. McKenzie, Jr., N. Jiang, X. Li, M. J. Wagner, D. P. Durkin, H. Chen, and D. Shuai. "Radical-Driven Decomposition of Graphitic Carbon Nitride Nanosheets: Light Exposure Matters," *Environmental Science & Technology* (September 2021), ACS Publications. doi: 10.1021/acs.est.1c03804

Moberg, D. R., and A. W. Jasper. "Permutationally Invariant Polynomial Expansions with Unrestricted Complexity," *Journal of Chemical Theory and Computation* (September 2021), ACS Publications. doi: 10.1021/acs.jctc.1c00352

October

Baroni, A., G. B. King, and S. Pastore. "Electroweak Currents from Chiral Effective Field Theory," *Few-Body Systems* (October 2021), SpringerLink. doi: 10.1007/s00601-021-01700-6

Fukami, K., R. Maulik, N. Ramachandra, K. Fukagata, and K. Taira. "Global Field Reconstruction from Sparse Sensors with Voronoi Tessellation-Assisted Deep Learning," *Nature Machine Intelligence* (October 2021), Springer Nature. doi: 10.1038/s42256-021-00402-2

Bucaro, A., C. Murphy, N. Ferrier, J. Insley, V. Mateevitsi, M. E. Papka, S. Rizzi, and J. Tan. "Instrumenting Multiphysics Blood Flow Simulation Codes for In Situ Visualization and Analysis," *2021 IEEE 11th Symposium on Large Data Analysis and Visualization (LDAV)* (October 2021), IEEE. doi: 10.1109/LDAV53230.2021.00018

Savira, P., T. Marrinan, and M. E. Papka. "Writing, Running, and Analyzing Large-Scale Scientific Simulations with Jupyter Notebooks," *2021 IEEE 11th Symposium on Large Data Analysis and Visualization (LDAV)* (October 2021), IEEE. doi: 10.1109/ldav53230.2021.00020

Bott, A. F. A., L. Chen, G. Boutoux, T. Caillaud, A. Duval, M. Koenig, B. Khiar, I. Lantuéjoul, L. Le-Deroff, B. Reville, R. Rosch, D. Ryu, C. Spindloe, B. Vauzour, B. Villette, A. A. Schekochihin, D. Q. Lamb, P. Tzeferacos, G. Gregori, and A. Casner. "Inefficient Magnetic-Field Amplification in Supersonic Laser-Plasma Turbulence," *Physical Review Letters* (October 2021), APS. doi: 10.1103/PhysRevLett.127.175002

Nagakura, H., A. Burrows, L. Johns, and G. M. Fuller. "Where, When, and Why: Occurrence of Fast-Pairwise Collective Neutrino Oscillation in Three-Dimensional Core-Collapse Supernova Models," *Physical Review D* (October 2021), APS. doi: 10.1103/PhysRevD.104.083025

Dzodzo, M. B. "Validation of Computational Fluid Dynamics Models for Industrial Applications," *2021 28th International Conference on Nuclear Engineering* (October 2021), ASME. doi: 10.1115/ICONE28-66712

Pham, B. Q., D. Datta, and M. S. Gordon. "PDG: A Composite Method Based on the Resolution of the Identity," *The Journal of Physical Chemistry A* (October 2021), ACS Publications. doi: 10.1021/acs.jpca.1c06186

Dettrick, S. A., D. C. Barnes, F. Ceccherini, L. Galeotti, S. A. Galkin, S. Gupta, K. Hubbard, O. Koshkarov, C. K. Lau, Y. Mok, A. Necas, B. S. Nicks, M. Onofri, J. Park, S. V. Putvinski, L. C. Steinhauer, K. Yakymenko, P. N. Yushmanov, T. Tajima, E. V. Belova, Z. Lin, W. Wang, and X. Wei. "Simulation of Equilibrium and Transport in Advanced FRCS," *Nuclear Fusion* (October 2021), IOP Publishing. doi: 10.1088/1741-4326/ac1e5f

Bollweg, D., J. Goswami, O. Kaczmarek, F. Karsch, S. Mukherjee, P. Petreczky, C. Schmidt, and P. Scior (HotQCD Collaboration). "Second Order Cumulants of Conserved Charge Fluctuations Revisited: Vanishing Chemical Potentials," *Physical Review D* (October 2021), APS. doi: 10.1103/PhysRevD.104.074512

Bhati, A. P., S. Wan, D. Alfe, A. R. Clyde, M. Bode, L. Tan, M. Titov, A. Merzky, M. Turilli, S. Jha, R. R. Highfield, W. Rocchia, N. Scafuri, S. Succi, D. Kranzlmuller, G. Mathias, D. Wifling, Y. Donon, A. Di Meglio, S. Vallecorsa, H. Ma, A. Trifan, A. Ramanathan, T. Brettin, A. Partin, F. Xia, X. Duan, R. Stevens, and P. V. Coveney. "Pandemic Drugs at Pandemic Speed: Infrastructure for Accelerating COVID-19 Drug Discovery with Hybrid Machine Learning- and Physics-Based Simulations on High-Performance Computers," *Interface Focus* (October 2021), The Royal Society. doi: 10.1098/rsfs.2021.0018

Trifan, A., D. Gorgun, Z. Li, A. Brace, M. Zvyagin, H. Ma, A. Clyde, D. Clark, M. Salim, D. J. Hardy, T. Burnley, L. Huang, J. McCalpin, M. Emani, H. Yoo, J. Yin, A. Tsaris, V. Subbiah, T. Raza, J. Liu, N. Trebesch, G. Wells, V. Mysore, T. Gibbs, J. Phillips, S. C. Chennubhotla, I. Foster, R. Stevens, A. Anandkumar, V. Vishwanath, J. E. Stone, E. Tajkhorshid, S. A. Harris, and A. Ramanathan. "Intelligent Resolution: Integrating Cryo-EM with AI-Driven Multi-Resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action," *SC '21: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis.* doi: 10/2021,IEEE,10.1101/2021.10.09.463779

Wood, B. C., J. B. Varley, K. E. Kweon, P. Shea, A. T. Hall, A. Grieder, M. Ward, V. P. Aguirre, D. Rigling, E. Lopez Ventura, C. Stancill, and N. Adelstein. "Paradigms of Frustration in Superionic Solid Electrolytes," *Royal Society* (October 2021), The Royal Society. doi: 10.1098/rsta.2019.0467

Zhang, C., and A. A. Chien. "Scheduling Challenges for Variable Capacity Resources," JSSPP 2021 (October 2021), Springer International Publishing. doi: 10.1007/978-3-030-88224-2_10

Jackson, N., and G. Sivaraman. “Coarse-Grained Density Functional Theory Predictions via Deep Kernel Learning,” *Creative Commons* (October 2021), ScienceGate. doi: 10.33774/chemrxiv-2021-bkdfv

Summerfield, N., B.-N. Lu, C. Plumberg, D. Lee, J. Noronha-Hostler, and A. Timmins. “16 O 16 O Collisions at Energies Available at the BNL Relativistic Heavy Ion Collider and at the CERN Large Hadron Collider Comparing Œ± Clustering versus Substructure,” *Physical Review C* (October 2021), APS. doi: 10.1103/PhysRevC.104.L041901

Song, Y. H., Y. Kim, N. Li, B.-N. Lu, R. He, D. Lee. “Quantum Many-Body Calculations Using Body-Centered Cubic Lattices,” *Physical Review C* (October 2021), APS. doi: 10.1103/PhysRevC.104.044304

Kang, S., E. M. Constantinescu, H. Zhang, and R. L. Jacob. “Mass-Conserving Implicit–Explicit Methods for Coupled Compressible Navier–Stokes Equations,” *Computer Methods in Applied Mechanics and Engineering* (October 2021), Elsevier. doi: 10.1016/j.cma.2021.113988

Luna, A., J. Bernanke, K. Kim, N. Aw, J. D. Dworkin, J. Cha, and J. Posner. “Maturity of Gray Matter Structures and White Matter Connectomes, and Their Relationship with Psychiatric Symptoms in Youth,” *PubMed* (October 2021), National Library of Medicine. doi: 10.1002/hbm.25565

November

Shen, H., E. A. Huerta, E. O’Shea, P. Kumar, and Z. Zhao. “Statistically-Informed Deep Learning for Gravitational Wave Parameter Estimation,” *Machine Learning: Science and Technology* (November 2021), IOP Science. doi: 10.1088/2632-2153/ac3843

Qiao, Z., X. Shi, M. Wojcik, and L. Assoufid. “High-Resolution Scanning Coded-Mask-Based X-ray Multi-Contrast Imaging and Tomography,” *Journal of Imaging* (November 2021), MDPI. doi: 10.3390/jimaging7120249

Hidayetoglu, M., T. Bicer, S. Garcia de Gonzalo, B. Ren, D. Gursoy, R. Kettimuthu, I. Foster, and W.-M. W. Hwu. “MemXCT: Design, Optimization, Scaling, and Reproducibility of X-ray Tomography Imaging,” *IEEE Transactions on Parallel and Distributed Systems (Early Access)* (November 2021), IEEE. doi: 10.1109/TPDS.2021.3128032

Liu, Z., A. Ali, P. Kenesei, A. Miceli, H. Sharma, and N. Schwarz. “Bridging Data Center AI Systems with Edge Computing for Actionable Information Retrieval,” *2021 3rd Annual Workshop on Extreme-Scale Experiment-in-the-Loop Computing (XLOOP)* (November 2021), IEEE. doi: 10.1109/XLOOP54565.2021.00008

Waters, D., C. MacLean, D. Bonachea, and P. Hargrove. “Demonstrating UPC++/Kokkos Interoperability in a Heat Conduction Simulation (Extended Abstract),” *The 4th Annual Parallel Applications Workshop* (November 2021), eScholarship. doi: 10.25344/S4630V

Kamil, A., and D. Bonachea. “Optimization of Asynchronous Communication Operations through Eager Notifications,” *The 4th Annual Parallel Applications Workshop, Alternatives To MPI+X (PAW-ATM)* (November 2021), eScholarship. doi: 10.25344/S42C71

Mondal, S., G. M. Magnotti, B. Lusch, R. Maulik, and R. Torelli. “Machine Learning-Enabled Prediction of Transient Injection Map in Automotive Injectors with Uncertainty Quantification,” *ASME 2021 Internal Combustion Engine Division Fall Technical Conference* (November 2021), ASME. doi: 10.1115/ICEF2021-67888

Bear, S., D. Parkinson, L. Gerhardt, M. Sibony, and B. Enders. “ALS Share, a Lightweight Data Sharing Service for a Synchrotron Radiation Facility,” *2021 3rd Annual Workshop on Extreme-Scale Experiment-in-the-Loop Computing (XLOOP)* (November 2021), IEEE. doi: 10.1109/xloop54565.2021.00006

Liu, X., R. Tom, S. Gao, and N. Marom. “Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors,” *The Journal of Physical Chemistry C* (November 2021), ACS Publications. doi: 10.1021/acs.jpcc.0c08160

Dekens, W., L. Andreoli, J. de Vries, E. Mereghetti, and F. Oosterhof. “A Low-Energy Perspective on the Minimal Left-Right Symmetric Model,” *Journal of High Energy Physics* (November 2021), Springer Nature. doi: 10.1007/JHEP11(2021)127

Wurtz, J., and D. Lykov. “Fixed-Angle Conjectures for the Quantum Approximate Optimization Algorithm on Regular MaxCut Graphs,” *Physical Review A* (November 2021), APS Physics. doi: 10.1103/physreva.104.052419

Zhao, D., R. Betti, and H. Aluie. “Scale Interactions and Anisotropy in Rayleigh-Taylor Turbulence,” *Journal of Fluid Mechanics* (November 2021), Cambridge University Press. doi: 10.1017/jfm.2021.902

Jain, A.,J. M. Cole, A. Vazquez-Mayagoitia, and M. Sternberg. “Modeling Dark- and Light-Induced Crystal Structures and Single-Crystal Optical Absorption Spectra of Ruthenium-Based Complexes That Undergo SO2-Linkage Photoisomerization,” *The Journal of Chemical Physics* (November 2021), AIP Publishing. doi: 10.1063/5.0077415

BezJ. L., H. Tang, B. Xie, D. Williams-Young, R. Latham, R. Ross, S. Oral, and S. Byna. “I/O Bottleneck Detection and Tuning: Connecting the Dots Using Interactive Log Analysis,” *2021 IEEE/ACM Sixth International Parallel Data Systems Workshop (PDSW)* (November 2021), IEEE. doi: 10.1109/PDSW54622.2021.00008

Ward, L., G. Sivaraman, J. G. Pauloski, Y. Babuji, R. Chard, N. Dandu, P. C. Redfern, R. S. Assary, K. Chard, L. A. Curtiss, R. Thakur, and I. Foster. “Colmena: Scalable Machine-Learning-Based Steering of Ensemble Simulations for High Performance Computing,” *2021 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC)* (November 2021), IEEE. doi: 10.1109/MLHPC54614.2021.00007

Liao, C., P.-H. Lin, G. Verma, T. Vanderbruggen, M. Emani, Z. Nan, X. Shen. “HPC Ontology: Towards a Unified Ontology for Managing Training Datasets and AI Models for High-Performance Computing,” *2021 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC)* (November 2021), IEEE. doi: 10.1109/MLHPC54614.2021.00012

Kwack, J. H., J. Tramm, C. Bertoni, Y. Ghadar, B. Homerding, E. Rangel, C. Knight, and S. Parker. “Evaluation of Performance Portability of Applications and Mini-Apps across AMD, Intel, and NVIDIA GPUs,” *2021 International Workshop on Performance, Portability and Productivity in HPC (P3HPC)* (November 2021), IEEE. doi: 10.1109/P3HPC54578.2021.00008

Dufek, A. S., R. Gayatri, N. Mehta, D. Doerfler, B. Cook, Y. Ghadar, and C. DeTar. “Case Study of Using Kokkos and SYCL as Performance-Portable Frameworks for Milc-Dslash Benchmark on NVIDIA, AMD, and Intel GPUs,” *2021 International Workshop on Performance, Portability, and Productivity in HPC (P3HPC)* (November 2021), IEEE. doi: 10.1109/p3hpc54578.2021.00009

Ko, H.-Y., B. Santra, and R. A. DiStasio, Jr. “Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaric–Isoenthalpic and Isobaric–Isothermal Ensembles,” *Journal of Chemical Theory and Computation* (November 2021), ACS Publications. doi: 10.1021/acs.jctc.0c01194

Egele, R., P. Balaprakash, I. Guyon, V. Vishwanath, F. Xia, R. Steven, and Z. Liu. “AgEBO-Tabular: Joint Neural Architecture and Hyperparameter Search with Autotuned Data-Parallel Training for Tabular Data,” *SC ’21: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (November 2021), ACM Digital Library. doi: 10.1145/3458817.3476203

Liu, Z., M. Fang, J. George, L.-J. Meng, and A. Di Fulvio. “Neutron Tomography of Spent Fuel Casks,” *Journal of Signal Processing Systems* (November 2021), Springer Nature. doi: 10.1007/s11265-021-01706-7

Simini, F., G. Barlacchi, M. Luca, and L. Pappalardo. “A Deep Gravity Model for Mobility Flows Generation,” *Nature Communications* (November 2021), Springer Nature. doi: 10.1038/s41467-021-26752-4

Holl, M., R. Kanungo, Z. H. Sn, G. Hagen, J. A. Lay, A. M. Moro, P. Navrátil, T. Papenbrock, M. Alcorta, D. Connolly, B. Davids, A. Diaz Varela, M. Gennari, G. Hackman, J. Henderson, S. Ishimoto, A. I. Kilic, R. Krücken, A. Lennarz, J. Liang, J. Measures, W. Mittig, O. Paetkau, A. Psaltis, and S. Quaglioni. “Proton Inelastic Scattering Reveals Deformation in 8He,” *Physics Letters B* (November 2021), Elsevier. doi: 10.1016/j.physletb.2021.136710

Ahn, J., I. Hong, G. Lee, H. Shin, A. Benali, and Y. Kwon. “Metastable Metallic Phase of a Bilayer Blue Phosphorene Induced by Interlayer Bonding and Intralayer Charge Redistributions,” *The Journal of Physical Chemistry Letters* (November 2021), ACS Publications. doi: 10.1021/acs.jpclett.1c03045

Lee, E. M. Y., A. Yu, J. J. de Pablo, and G. Galli. “Stability and Molecular Pathways to the Formation of Spin Defects in Silicon Carbide,” *Nature Communications* (November 2021), Springer Nature. doi: 10.1038/s41467-021-26419-0

Strano, E., F. Simini, M. De Nadai, T. Esch, and M. Marconcini. “The Agglomeration and Dispersion Dichotomy of Human Settlements on Earth,” *Scientific Reports* (November 2021), Springer Nature. doi: 10.1038/s41598-021-02743-9

Pauloski, J. G., Q. Huang, L. Huang, S. Venkataraman, K. Chard, I. Foster, and Z. Zhang. “KAISA: An Adaptive Second-Order Optimizer Framework for Deep Neural Networks,” *SC ’21: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis* (November 2021), ACM Digital Library. doi: 10.1145/3458817.3476152

Li, A., B. Fang, C. Granade, G. Prawiroatmodjo, B. Heim, M., Roetteler, and S. Krishnamoorthy. “SV-sim: Scalable PGAS-Based State Vector Simulation of Quantum Circuits,” *SC ’21: Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis* (November 2021), ACM Digital Library. doi: 10.1145/3458817.3476169

December

Maulik, R., and G. Mengaldo. “PyParSVD: A Streaming, Distributed, and Randomized Singular-Value-Decomposition Library,” *2021 7th International Workshop on Data Analysis and Reduction for Big Scientific Data (DRBSD-7)* (December 2021), IEEE. doi: 10.1109/drbsd754563.2021.00007

Guo, H., P. Poths, P. Sautet, and A. N. Alexandrova. “Oxidation Dynamics of Supported Catalytic Cu Clusters: Coupling to Fluxionality,” *American Chemical Society* (December 2021), ACS Publications. doi: 10.1021/acscatal.1c04100

Verma, G., M. Emani, C. Liao, P.-H. Lin, T. Vanderbruggen, X. Shen, and B. Chapman. “HPCFAIR: Enabling FAIR AI for HPC Applications,” *2021 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC)* (December 2021), IEEE. doi: 10.1109/MLHPC54614.2021.00011

Navrátil, P., “Translationally Invariant Matrix Elements of General One-Body Operators,” *Physical Review C* (December 2021), APS. doi: 10.1103/PhysRevC.104.064322

Fu, L., M. Karp, S. T. Bose, P. Moin, and J. Urzay. “Shock-Induced Heating and Transition to Turbulence in a Hypersonic Boundary Layer,” *Journal of Fluid Mechanics* (December 2021), Cambridge University Press. doi: 10.1017/jfm.2020.935

Vartanyan, D., M. S. B. Coleman, and A. Burrows. “The Collapse and Three-Dimensional Explosion of Three-Dimensional Massive-Star Supernova Progenitor Models,” *Monthly Notices of the Royal Astronomical Society* (December 2021), Oxford University Press. doi: 10.1093/mnras/stab3702

Goc, K. A., O. Lehmkuhl, G. I. Park, S. T. Bose, and P. Moin. “Large Eddy Simulation of Aircraft at Affordable Cost: A Milestone in Computational Fluid Dynamics,” *FLOW Applications of Fluid Mechanics* (December 2021), Cambridge University Press. doi: 10.1017/flo.2021.17

Ramesh, S., R. Ross, M. Dorier, A. Malony, P. Carns, and K. Huck. “SYMBIOMON: A High-Performance, Composable Monitoring Service,” *2021 IEEE 28th International Conference on High Performance Computing, Data, and Analytics (HiPC)* (December 2021), IEEE. doi: 10.1109/HiPC53243.2021.00047

Albergo, M. S., G. Kanwar, S. Racaniere, D. J. Rezende, J. M. Urban, D. Boyda, K. Cranmer, D. C. Hackett, and P. E. Shanahan. “Flow-Based Sampling for Fermionic Lattice Field Theories,” *Physical Review D* (December 2021), APS. doi: 10.1103/PhysRevD.104.114507

Antypas, K. B., D. J. Bard, J. P. Blaschke, R. S. Canon, B. Enders, M. A. Shankar, S. Somnath, D. Stansberry, T. D. Uram, and S. R. Wilkinson. “Enabling Discovery Data Science through Cross-Facility Workflows,” *2021 IEEE International Conference on Big Data (Big Data)* (December 2021), IEEE. doi: 10.1109/bigdata52589.2021.9671421

Tang, H., S. Byna, N. A. Petersson, and D. McCallen. “Tuning Parallel Data Compression and I/O for Large-Scale Earthquake Simulation,” *2021 IEEE International Conference on Big Data (Big Data)* (December 2021), IEEE. doi: 10.1109/bigdata52589.2021.9671876

Sun, Z. H., G. Hagen, G. R. Jansen, and T. Papenbrock. “Effective Shell-Model Interaction for Nuclei “Southeast” of 100Sn,” *Physical Review C* (December 2021), APS. doi: 10.1103/PhysRevC.104.064310

Shi, Y., M. Rabbani, A. Vazquez-Mayagoitia, J. Zhao, and W. A. Saidi. “Controlling the Nucleation and Growth of Ultrasmall Metal Nanoclusters with MoS2 Grain Boundaries,” *Nanoscale* (December 2021), Royal Society of Chemistry. doi: 10.1039/d1nr07836d

Werner, G. R., and D. A. Uzdensky. “Reconnection and Particle Acceleration in Three-Dimensional Current Sheet Evolution in Moderately Magnetized Astrophysical Pair Plasma,” *Journal of Plasma Physics* (December 2021), Cambridge University Press. doi: 10.1017/S0022377821001185

Linker, T., Y. Wang, A. Mishra, D. Kamal, Y. Cao, R. K. Kalia, A. Nakano, R. Ramprasad, F. Shimojo, G. Sotzing, and P. Vashishta. “Deep Well Trapping of Hot Carriers in a Hexagonal Boron Nitride Coating of Polymer Dielectrics,” *ACS Applied Materials & Interfaces* (December 2021), ACS Publications. doi: 10.1021/acsami.1c14587

Andrade, T., L. Salo, J. Aurrekoetxea, J. Bamber, K. Clough, R. Croft, E. de Jong, A. Drew, A. Duran, P. Ferreira, P. Figueras, H. Finkel, T. Frana, B.-X. Ge, C. Gu, T. Helfer, J. Jäykkä, C. Joana, M. Kunesch, K. Kornet, E. Lim, F. Muia, Z. Nazari, M. Radia, J. Ripley, P. Shellard, U. Sperhake, D. Traykova, S. Tunyasuvunakool, Z. Wang, J. Widdicombe, and K. Wong. “GRChombo: An Adaptable Numerical Relativity Code for Fundamental Physics,” *Journal of Open Source Software* (December 2021), The Open Journal. doi: 10.21105/joss.03703

Gnech, A., C. Adams, N. Brawand, G. Carleo, A. Lovato, and N. Rocco. “Nuclei with Up to A = 6 Nucleons with Artificial Neural Network Wave Functions,” *Few-Body Systems* (December 2021), Springer. doi: 10.1007/s00601-021-01706-0

Liu, Q., W. Jiang, Z. Yang, and Z. Zhang. “An Environmentally Benign Electrolyte for High Energy Lithium Metal Batteries,” *ACS Applied Materials & Interfaces* (December 2021), APS. doi: 10.1021/acsami.1c19124

Yang, H., M. Govoni, A. Kundu, and G. Galli. “Combined First-Principles Calculations of Electron–Electron and Electron–Phonon Self-Energies in Condensed Systems,” *CCC RightsLink* (December 2021), American Chemical Society (ACS). doi: 10.1021/acs.jctc.1c00605

Williams-Young, D. B., A. Bagusetty, W. A. de Jong, D. Doerfler, H. J. J. van Dam, Å. Vázquez-Mayagoitia, T. L. Windus, and Chao, Yanga. “Achieving Performance Portability in Gaussian Basis Set Density Functional Theory on Accelerator-Based Architectures in NWChemEx,” *Parallel Computing* (December 2021), Science Direct. doi: 10.1016/j.parco.2021.102829

About the Argonne Leadership Computing Facility

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

About Argonne National Laboratory

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

Availability of this Report (ANL/ALCF-22/1)

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

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

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

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

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

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

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

ALCF Leadership: Michael E. Papka (Division Director), Jini Ramprakash (Deputy Division Director), Katherine Riley (Director of Science), Kalyan Kumaran (Director of Technology), Mark Fahey (Director of Operations), and Susan Coghlan (ALCF-X Project Director)

Editorial Team: Beth Cerny, Jim Collins, Nils Heinonen, Logan Ludwig, and Laura Wolf

Design and production: Sandbox Studio, Chicago

CONTACT
media@alcf.anl.gov
alcf.anl.gov

U.S. DEPARTMENT OF ENERGY

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