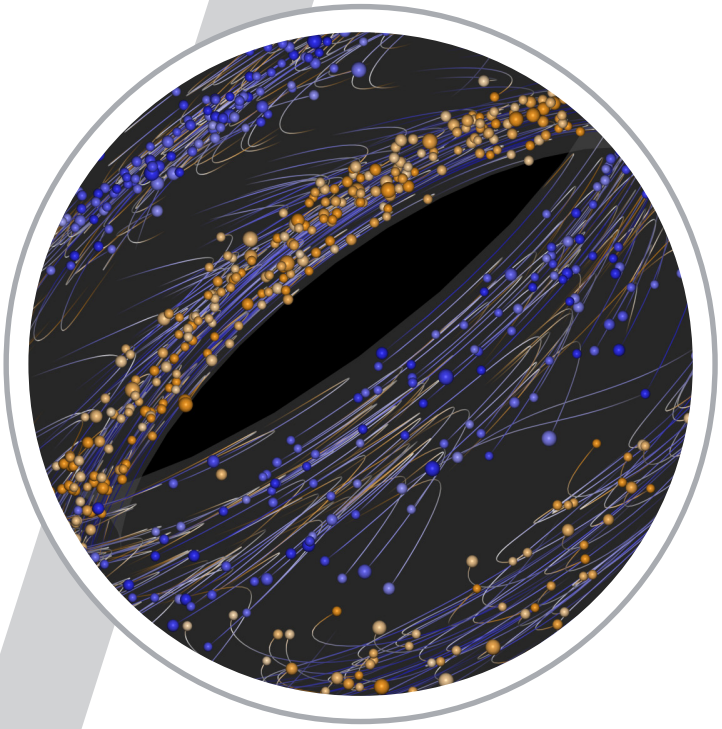
# 2013 ANNUAL REPORT

ARGONNE **LEADERSHIP COMPUTING** FACILITY



Argonne NATIONAL LABORATORY

# ARGONNE LEADERSHIP COMPUTING FACILITY
# 2013 ANNUAL REPORT

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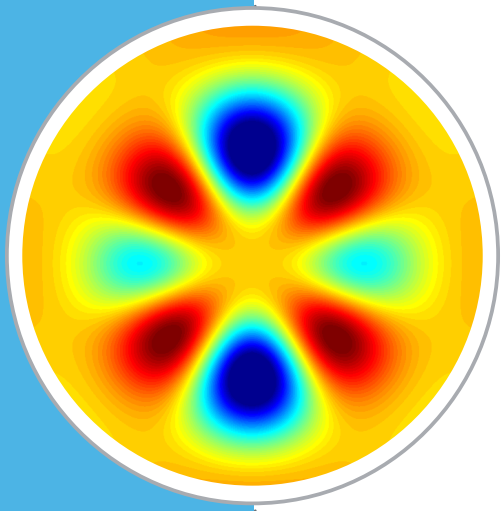
# ABOUT ALCF

The Argonne Leadership Computing Facility provides researchers from national laboratories, academia, and industry with access to high-performance computing capabilities to enable breakthrough science and engineering. Supported by the U.S. Department of Energy Office of Science, the ALCF is one of two leadership computing facilities in the nation dedicated to open science.



# MISSION

The ALCF's mission is to accelerate major scientific discoveries and engineering breakthroughs by designing and providing world-leading computing facilities in partnership with the computational science community.

# 2013 **BY THE NUMBERS**

**4.79** billion core-hours of total compute time

**1,150** facility users

**300+** active projects

**150+** publications

DIRECTOR'S MESSAGE

# **LEADERSHIP COMPUTING** PAVES THE WAY FOR SCIENTIFIC DISCOVERIES

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

Ten years ago the DOE's Advanced Scientific Computing Research (ASCR) program founded the Leadership Computing Facility to lead the world in open scientific computing. It was a huge investment in the nation's scientific and technological future, inspired by a growing demand for capability computing and its impact on science and engineering.

ASCR's Leadership Computing Facility, or LCF, operates two world-class centers, at Argonne National Laboratory and at Oak Ridge National Laboratory, and deploys two diverse high-performance computer architectures that are 10 to 100 times more powerful than systems typically available for open scientific research.

As a new generation of systems is deployed, the LCF serves as the premier source of petaflops dedicated to tackling the largest and most complex problems in biology, fusion energy, astrophysics, particle physics, and more. Strategically, it ranks among the top U.S. scientific facilities needed over the next 20 years to deliver impactful science, help inform policy decisions, and advance innovation in far reaching topics such as energy assurance, ecological sustainability, and global security.

Our focus at the Argonne Leadership Computing Facility (ALCF) this year was the launch of our newest production system, a 48-rack IBM Blue Gene/Q system called Mira. This upgrade to a 10-petaflops system is the direct result of a five-year partnership between Argonne and Lawrence Livermore national laboratories, and IBM.

On April 9, Mira officially replaced Intrepid as the ALCF's major production resource. Meanwhile, Intrepid continued to support numerous projects and run as a full production system until it was retired on December 31, concluding yet another era in Argonne's computing history that now spans more than three decades.

Mira's unique architecture represents a new class of capabilities for ALCF's user community. Early in its deployment, ALCF worked with researchers on 15 "early science" projects to ensure science on day one. Now our users are getting more science per core in their quests to design effective pharmaceuticals faster, to probe the cosmic structure of the Dark Universe, and to develop quieter, more fuel-efficient wind turbines and jet engines.

Moving forward into 2014 the LCF has awarded a record number of core-hours to the largest number of research projects ever at ALCF. Ten years ago, the U.S. decided to lead the world with the founding of the LCF, and today the entire world is benefitting from this leadership. There is no facility better positioned to enable open science discoveries than the LCF, and we at the ALCF dedicate ourselves every day to this very important mission.

# ALCF LEADERSHIP: YEAR IN REVIEW

SUSAN COGHLAN

Even before Mira entered production mode in April 2013, we had begun preparing for our next-generation leadership computing system (ALCF-3). With the approval of Mission Need and Critical Decision-0 (CD-0) in January 2013, the ALCF-3 project was initiated and our project team began working diligently to develop and prepare the preliminary plan and documentation. In parallel with this effort, DOE formed the CORAL project, a collaboration between Argonne, Oak Ridge, and Lawrence Livermore national laboratories, to develop a joint competitive request for proposal (RFP) for the DOE's next three state-of-the-art leadership supercomputers (one for each laboratory) for delivery in 2017-2018. The Design Review and subsequent RFP Review helped us to evaluate and fine-tune project plans. In September, the ALCF-3 CD-1/3a Review addressed the acquisition strategy, alternatives analysis, preliminary schedule, and project plan. With the approval of CD-1/3a in October, the ALCF-3 project was given the green light to solicit proposals for long-lead procurements, including the RFP release, selection, and contract negotiations for the computing system. In 2014, we look forward to evaluating and selecting the winning set of proposals for the RFP, negotiating the contractual agreement and statement of work with our selected vendor, and finalizing the baseline documents for the ALCF-3 project.

**— Susan Coghlan, Deputy Director**

PAUL MESSINA

The ALCF had a memorable year in 2013. We wrapped up an extremely productive five-year run on Intrepid, while also beginning the next era of supercomputing at the ALCF with the launch of Mira. Since entering production mode in April, Mira has consistently enabled researchers to take on larger and more complex problems than ever before, usually porting applications from other systems with modest effort. In 2013, the ALCF delivered 4.79 billion core-hours of compute time, with 2.61 billion of those core-hours being used by capability jobs. The science done on our machines produced more than 150 publications, spanning a broad spectrum of fields. Additionally, we organized and ran the inaugural Argonne Training Program on Extreme-Scale Computing (ATPESC), a two-week training program funded by DOE that is designed to train the next generation of supercomputer users. We are eager to see the breakthroughs Mira will enable in 2014, its first full year of production operation.

**— Paul Messina, Director of Science**

BILL ALLCOCK

2013 was a busy year of transition for the ALCF Operations Team. We prepared Mira for full production, while also beginning the process of shutting down Intrepid. Besides being a large, complicated task, the decommissioning effort was a little sad since Intrepid was our first production machine and she ran like a champ for us. Additionally, our team began a major storage expansion to provide more space on Mira and a better than 50% bandwidth increase to the Mira storage system. This work also involves a complete refresh of the HPSS hardware, which will result in a more than 3x increase in bandwidth to the disk cache and 50% bandwidth increase to tape. In 2014, we look forward to improving the operational efficiency of Mira and completing the storage upgrades.

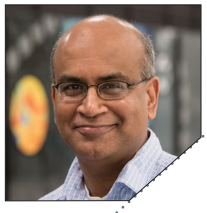
**— Bill Allcock, Director of Operations**

At the ALCF, User Experience cultivates an understanding of the user's story: who they are, what they need to succeed, how their contributions impact the world, and how we can best help them discover. This understanding enables us to remove crucial roadblocks and provide information to help users get the most out of our resources. In 2013, we integrated checklists into our communications with users, improving message clarity and response rate. In tandem with the launch of Mira, ALCF worked as a team to deliver the critical documentation needed to run on our new resources. We also executed an outreach strategy to get the word out about who we are and how we can advance science and engineering. In 2014, I look forward to supporting world-class scientists from a myriad of organizations and working alongside the best and brightest leadership computing staff in the world.

RICHARD COFFEY

**— Richard Coffey, Director of User Experience**

The Performance Engineering Team played an important role in helping Mira hit the ground running in 2013. We ensured that all of the requisite programming models, tools, debuggers, and libraries were available for use on day one. This included writing detailed documentation and a few conference papers to help users understand how to take advantage of these resources. We also helped ease the transition from Intrepid to Mira by working directly with users at our Mira Performance Boot Camp in May. While the launch of Mira was the big news of 2013, we we also began preparing for the next-generation ALCF supercomputer. As part of the CORAL request for proposal, our group collaborated to write the technical requirements for several sections, including the development of new benchmarks to address emerging data-centric workloads. In 2014, we look forward to continuing our work to prepare for ALCF-3. We will also be supporting current and future ALCF users through our ongoing participation in DOE research programs aimed at accelerating the development of technologies critical to extreme-scale computing.



KALYAN KUMARAN

**— Kalyan Kumaran, Manager, Performance Engineering**

We successfully moved operations from Eureka to Tukey, the temporary visualization and analysis IBM Blue Gene/Q resource. Our team worked with INCITE scientists to produce visualizations for a Gordon Bell finalist paper, and animations for the SC13 Visualization Showcase and the AAAS Science Film Showcase. We provided expertise that dramatically improved I/O performance for one of our industrial science teams (also an INCITE project), leading to an animation showcased in the DOE and Kitware booths at SC13. The improved output scheme is now incorporated into the commercial simulation tool that they use. In the coming year we will be working toward developing a groundbreaking new capability to interactively explore trillion-particle datasets equivalent to million-cubed volumes in voxel space. We will also be procuring our next-generation visualization and analysis leadership resource.

MARK HERELD

**— Mark Hereld, Manager, Visualization and Data Analysis**

# MIRA DEDICATION CEREMONY
## Marks New Era at the ALCF

On July 1, U.S. Senator Dick Durbin (D-IL) led the dedication of Mira at the Argonne Leadership Computing Facility, underscoring the importance of high-performance computing to scientific research, industrial innovation, and our nation's economic future.

"Argonne National Laboratory is one of Illinois' and the country's great assets," Durbin said. "Mira ensures the lab remains a linchpin of scientific research, enabling researchers to tackle extremely complex challenges ranging from improving combustion efficiency in car engines to modeling the progression of deadly diseases in the human body. High-performance computing is crucial to U.S. economic growth and competitiveness, saving time, money and energy, boosting our national security and strengthening our economy. If the United States is to remain a leader in the 21st century, we need to continue investing in the science and innovation that will address our growing energy and environmental demands while building the industries of the future."

Argonne Director Eric Isaacs, Associate Laboratory Director Rick Stevens, and David Turek, Vice President for Exascale Computing at IBM, also spoke at the dedication ceremony.

*U.S. Senator Dick Durbin (D-IL)*

"High-performance computing is crucial to U.S. economic growth and competitiveness, saving time, money and energy, boosting our national security and strengthening our economy."

*From left to right: Joanna Livengood, Manager of the U.S. Department of Energy's Argonne Site Office; David Turek, Vice President for Exascale Computing at IBM; Rick Stevens, Argonne Associate Laboratory Director for Computing, Environment and Life Sciences; U.S. Senator Dick Durbin (D-IL); Eric Isaacs, Argonne Director; Donald Levy, University of Chicago Vice President for Research and for National Laboratories.*

"High-performance computing is a critical technology, both for science and for industry," Isaacs said. "Mira will help U.S. researchers to maintain a competitive edge in the development of new products and services. This is a great addition to Argonne's unique suite of Department of Energy user facilities, and I am sure Mira will serve as yet another magnet for innovation in Illinois."

Mira, an IBM Blue Gene/Q system, consists of 48 racks of computers, 786,432 processors, and 768 terabytes of memory. The machine is capable of 10 quadrillion calculations per second – making it one of the fastest supercomputers in the world. To put those capabilities in perspective, Mira is 20 times faster than its IBM Blue Gene/P predecessor at the ALCF, Intrepid, which was ranked as the third fastest computer in the world when it was installed in 2008.

Mira also represents a great step forward in green computing. With a highly efficient water-cooling system and innovative chip designs, Mira operates five times more efficiently than Intrepid.

*Rick Stevens, Argonne Associate Laboratory Director for Computing, Environment and Life Sciences*

*The dedication ceremony was attended by invited guests from DOE, Argonne, and the HPC community.*

# Early Science Program Helps Ready MIRA for **SCIENTIFIC DISCOVERIES**

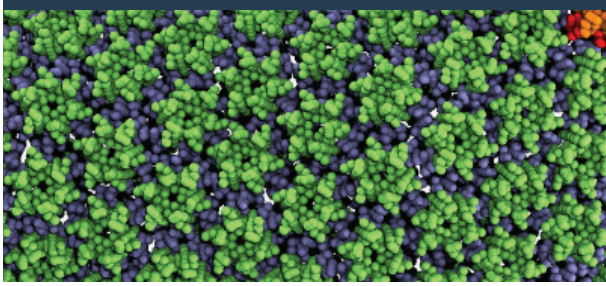
The ALCF's Early Science Program (ESP) came to a close at the end of 2013, completing a three-year run that successfully prepared Mira for science on day one.

Launched in October 2010, the intent of ESP was to use the critical pre-production time period on Mira to prepare key applications for the architecture and scale of the new supercomputer and to solidify the necessary libraries and infrastructure. In addition to their plans to deliver new science, the 16 ESP projects were chosen based on their state-of-the-art, petascale applications, which were especially well suited to exploit the unique characteristics of Blue Gene/Q architecture.

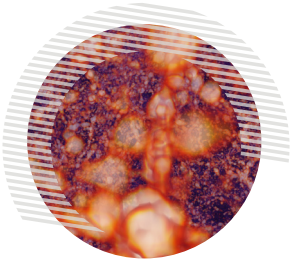
The dedicated Early Science period lasted only a few months (between machine acceptance in December 2012 and commencement of production in April 2013), during which the 16 ESP projects aimed to burn over 2 billion core-hours on Mira. It was essential that the projects were ready to run when the clock started ticking. This was made possible by the program's long lead-time and having dedicated postdoctoral appointees and ALCF staff help advance most projects. Once Mira went online in April, ESP teams were able to continue using the system to pursue their scientific goals through the end of 2013.

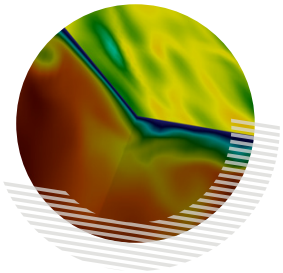
Over the course of three years, the ESP resulted in many successful outcomes including:

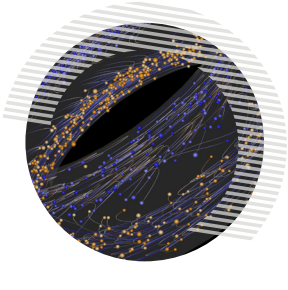
- A wide variety of applications were ported to Blue Gene/Q, all with significantly improved performance relative to Blue Gene/P or other previous-generation machines.
- Each of the 16 projects published technical reports to document the computational efforts and lessons learned in preparing the projects' applications to run on Mira. The reports are publicly available on the ALCF website.
- A majority of the ESP projects have transitioned into INCITE projects.
- The 11 postdocs assigned to ESP projects have advanced their careers as computational scientists significantly as a result of their work in the program.

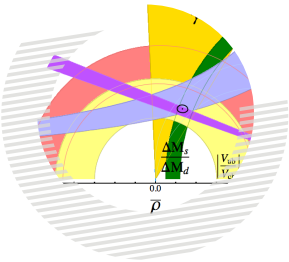


The 16 ESP projects pursued real scientific problems while simultaneously preparing key applications for the architecture and scale of Mira.









# Breaking New Ground with **Mira**

With Mira officially entering full production mode in April 2013, several projects began taking advantage of the system's vastly increased power and capabilities to run simulations of unprecedented scale and accuracy, allowing scientists to tackle larger and more complex problems than ever before. A few examples include:

### Lattice QCD

PI: Paul Mackenzie, Fermilab

The Lattice QCD research team has leveraged Mira to study the behavior of quarks and gluons in situations that are not possible in accelerator and cosmic ray experiments. With the IBM Blue Gene/Q system, the researchers were able to give quark-antiquark pairs their proper, very light masses for the first time, removing one of the largest remaining uncertainties involved in quantum chromodynamics calculations.

### Kinetic Simulations of Fusion Energy Dynamics at the Extreme Scale

PI: William Tang, Princeton Plasma Physics Laboratory

Mira has made it possible for researchers at Princeton Plasma Physics Laboratory to study large-scale tokamak fusion energy systems, such as ITER, in greater detail than ever before. Simulations on Mira led them to discover that the magnitude of plasma turbulent losses is up to 50% lower than indicated by earlier simulations carried out at much lower resolution and significantly shorter duration.

### Computing the Dark Universe

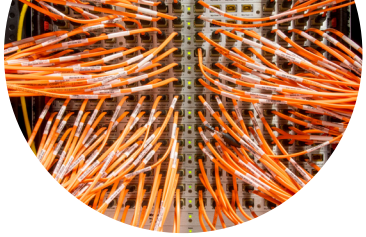
PI: Salman Habib, Argonne National Laboratory

An Argonne-led team used Mira to conduct the largest and most detailed simulations of the universe ever performed. This has given researchers the first simulations that are accurate enough to compare with the state-of-the-art sky surveys in studies into the nature of dark energy and dark matter.

### Direct Numerical Simulations of High Reynolds Number Turbulent Channel Flow

PI: Robert Moser, Universtiy of Texas at Austin

Researchers from University of Texas at Austin used Mira to study wall-bounded turbulence at an extraordinary level of detail with the largest production direct numerical simulations performed to date. This work is expected to lead to an improved understanding of the underlying physics and the creation of new tools for the reduction of drag.



# PASSING THE TORCH
# INTREPID TO MIRA

Much like personal computers, the average lifespan of a supercomputer is four to five years. In 2013, Intrepid, the ALCF's IBM Blue Gene/P supercomputer, hit the five-year mark, ending an impressive run of innovative computational research.

Ranked as the third fastest computer in the world when it debuted in 2008, Intrepid enabled researchers to accelerate studies of everything from advanced battery materials and climate models to supernovae and Parkinson's disease. The 557-teraflops system was decommissioned on December 31, 2013, but its legacy lives on in many of the ALCF's ongoing research projects.

Intrepid's successor, Mira, entered production mode in April 2013 and began handling the full ALCF workload in 2014. At 10 petaflops, the IBM Blue Gene/Q supercomputer has a peak speed 20 times faster than Intrepid.

With a vast majority of large-scale ALCF projects selected through the INCITE or ALCC allocation programs, many of the projects are multiyear efforts. Researchers often seek allocation renewals to continue their work from year to year, allowing research projects to evolve along with the facility and its increasingly powerful computing resources. In addition, many projects are so innovative and complex that it takes years to fully develop the software and achieve their goals.

## From Protein Structure Prediction to Protein Design

David Baker, head of the Institute of Protein Design at the University of Washington, has been tapping ALCF supercomputers for more than five years to advance the development of engineered proteins by creating and studying 3D models of protein structures at atomic-level resolution.

When Baker began using Intrepid in 2008, he gained access to a machine that would take his protein structure prediction work to new heights.

"It was really when we started using ALCF resources that we were able to take advantage of more and more sophisticated algorithms that were essentially able to dynamically relocate where we were focusing our research based on what we were finding," Baker said.

While Intrepid allowed Baker's team to successfully determine the structure of many proteins of biological interest, Mira is now enabling them to break new ground in protein design. With increased processing power and more memory per core, the researchers are able to model larger systems and store

thousands of different possible conformations, both of which are necessary for protein design. Currently, the team is working on designing peptides with future applications in possible protein therapeutics.

## Simulating Hydrogen Combustion in Industrial-Sized Pipes

University of Chicago Professor Alexei Khokhlov began using Intrepid in 2010 to advance the design of safer hydrogen fuel systems by studying the deflagration-to-detonation transition (DDT) process for hydrogen-oxygen mixtures.

DDT involves several physical processes, including chemical reactions, microscopic transport, turbulent fluid flows, and a wide range of temporal and spatial scales, which makes numerical modeling of these phenomena extremely computationally intensive.

"Intrepid was the first machine we could use to develop a new approach for direct numerical simulations of DDT in long pipes," said Khokhlov.

His first three years on ALCF systems were devoted to code development and validation on Intrepid, with early simulations showing excellent agreement with non-reactive experiments using carbon dioxide.

With the groundwork completed on Intrepid, Khokhlov's research team used Mira to study reactive hydrogen-oxygen mixtures, demonstrating the feasibility of first-principles DDT simulations in industrial-sized, meter-long pipes.

"These simulations are giving us an opportunity to study phenomena not observable in experiments," Khokhlov said. "Without Intrepid and Mira, this research would not exist."

## Nuclear Reactor Simulations Capture Industry Attention

Paul Fischer, senior computational scientist at Argonne, has also seen his research in nuclear reactor hydrodynamics take leaps and bounds during his time using ALCF resources.

The upward trajectory of the ALCF's computational capabilities can be seen in the progression of Fischer's simulations of nuclear reactor fuel assemblies. Prior to Intrepid, his research team was able to simulate a 7-pin fuel assembly. With Intrepid, they successfully simulated 19-pin, 37-pin, and, finally, full-scale 217-pin bundles.

Intrepid also enabled the first high-fidelity simulations of wire-wrapped fuel pins, which added to the accuracy of the simulations and helped to capture the attention of the nuclear engineering community. Fischer's work continues to improve and evolve on Mira, with his research team now collaborating with four industrial partners to simulate different kinds of fuel assemblies.

In addition to the groundbreaking nuclear reactor simulations, Fischer's team leveraged Intrepid to perform many so-called "hero calculations" that tested the limits of high-performance computing. This allowed them to achieve many firsts for Fischer's Nek5000 code, including running on 1 million cores and performing simulations that exceeded 1 billion grid points.

"What was considered a hero calculation in 2009 is now being done routinely on Mira to address real-world engineering questions," Fischer said. "It really shows you how the evolution of high-performance computing will continue to allow us to go into new places that we haven't been able to go before."

# TRAINING USERS FOR MIRA AND BEYOND

Each year, the ALCF offers a variety of workshops, conferences, and events to provide training and information for new, existing, and prospective ALCF users. In 2013, the focus was on preparing users to hit the ground running with Mira in its first year of operation. This included several expert-guided, hands-on training sessions on the tools, computational resources, and services available to users in support of scientific discovery.

### Getting Started Webinars (January 17, 18, 24, 25)

The ALCF offered several Getting Started videoconferences to provide users with information on ALCF services and resources, technical details on the IBM Blue Gene/Q architecture, and guided assistance in porting and tuning applications on Mira.

### Mira Community Conference (March 4-8)

In anticipation of Mira entering production mode in April, the ALCF hosted an international array of guests, including representatives from industry, other Blue Gene/Q user facilities, and researchers from many 2013 INCITE projects.

IBM provided a timely overview of key differences between the Blue Gene/P and the next-generation Blue Gene/Q. ALCF experts and software vendors teamed up to cover additional topics of interest for the transition to the new system, including code optimization, scaling, tools and debuggers, and parallel I/O.

### ESP Investigators Meeting (May 15-16)

Researchers from the 16 Early Science Program projects convened at the ALCF to discuss outcomes enabled by their participation in this preparatory program designed to ready Mira for production. Presentation topics included experiences and lessons learned from performing simulations of unprecedented scale, scope, and complexity.

### Mira Performance Boot Camp (May 21-24)

Researchers representing universities and institutions from across the nation and around the world participated in the ALCF's Mira Performance Boot Camp. For many, the primary goal of attending was to tap into the expertise of ALCF staff for assistance in improving their code's scalability to demonstrate computational readiness for a 2014 INCITE award. In support of this goal, the ALCF's annual scaling workshop was especially geared for and timed to coincide with efforts of teams preparing INCITE proposals.

The bulk of the four-day event was devoted to hands-on, one-on-one tuning of applications. ALCF experts also presented talks on topics of interest, including an overview of IBM Blue Gene/Q hardware and software architecture, manual code-tuning tips for peak performance, submission of ensemble jobs, and message-passing API on Mira. Tools and debugger developers were on hand to provide information and individualized assistance to attendees.

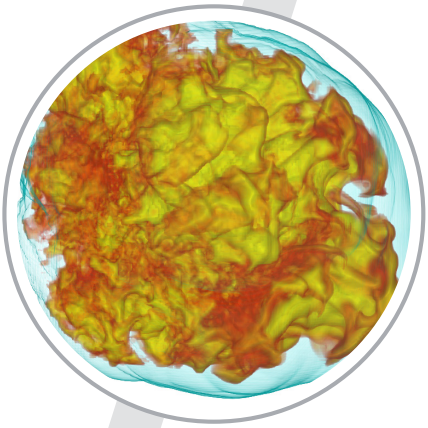
ATPESC Class of 2013

## Argonne Training Program on Extreme-Scale Computing (July 28 - August 9)

Organized and hosted by Argonne National Laboratory, this intensive two-week workshop served as a training course for future users of leadership-class supercomputers. The Argonne Training Program on Extreme-Scale Computing (ATPESC) provided hands-on training on the key skills, approaches, and tools to design, implement, and execute computational science and engineering applications on current high-end computing systems and the leadership-class computing systems of the future. As a bridge to that future, the training program was established to fill the gap that exists in the training computational scientists typically receive through formal education or other shorter courses.

The 2013 ATPESC class was comprised of 63 students, primarily PhD students and postdocs, representing a variety of disciplines and institutions from around the world. As part of their training, students were given access to some of today's most powerful supercomputing resources, such as Argonne's IBM Blue Gene/Q systems, Mira and Vesta; Oak Ridge's Cray XK7 system, Titan; and Georgia Tech's 264-node cluster, Keeneland.

Paul Messina, ALCF Director of Science, conceived the program as a way to grow the user community of today's leadership-class computing systems and of future resources expected to be available in 2017 and beyond. Course content was conceptualized, developed, and presented by teams of recognized HPC experts from national laboratories, computing institutions, academia, and industry. ATPESC received funding from the DOE's Office of Science for three consecutive summers—beginning with the 2013 program.



# EXPERTISE, RESOURCES & ALLOCATION PROGRAMS

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

**Catalysts** are computational scientists with domain expertise in areas such as chemistry, materials science, fusion, nuclear physics, plasma physics, computer science, engineering, and Earth science. Catalysts work directly with project PIs to maximize discovery and reduce time-to-solution.

**Performance Engineers** help users achieve optimal performance on ALCF resources by working with them to port, tune, and parallelize scientific applications and other software. This includes assessing and improving the algorithms used by applications and the techniques used to implement those algorithms.

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

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

**User Services and Outreach** provides frontline services and technical support to existing and potential ALCF users. The team also provides education and outreach to users, DOE, and the broader community.

# {2013 ACCOLADES}

**Adelchi Fabrocini Award >** Alessandro Lovato

Presented in recognition of the best doctoral thesis in nuclear physics, Lovato received the award for "Ab Initio Calculations on Nuclear Matter Properties Including the Effects of Three-Nucleons Interaction."

**Argonne Director's Award >** Katrin Heitmann, Ray Loy, Vitali Morozov, Paul Rich, Adam Scovel, William Scullin, and Tisha Stacey

Presented by Argonne National Laboratory, the team was recognized for outstanding contributions in system debugging and creative problem solving as part of the deployment and testing of Mira.

**SPECtacular Award >** Kalyan Kumaran

Presented by the Standard Performance Evaluation Corporation (SPEC), Kumaran was recognized for his outstanding work and leadership as chair of SPEC's High-Performance Group.

**Thomas Hart Benton Mural Medallion >** Paul Messina

Presented by Indiana University, Messina was honored for his significant contributions to high-performance computing. The medallion recognizes individuals who embody the values of the university and the universal academic community.

**Thomas Kuhn Paradigm Shift Award >** Anatole von Lilienfeld

Presented by OpenEye Scientific Software, von Lilienfeld was recognized for his talk "Quantum Machine: Supervised Learning of Schrodinger's Equation in Chemical Compound Space" at the American Chemical Society National Meeting.

**Young Achiever in Scalable Computing >** Jeff Hammond

Presented by the IEEE Technical Committee on Scalable Computing, Hammond was recognized for his contributions to computational chemistry applications, including NWChem and MADNESS, and for his work on partitioned global address space.

ALCF's staff, research, and resources recieved numerous accolades in 2013.

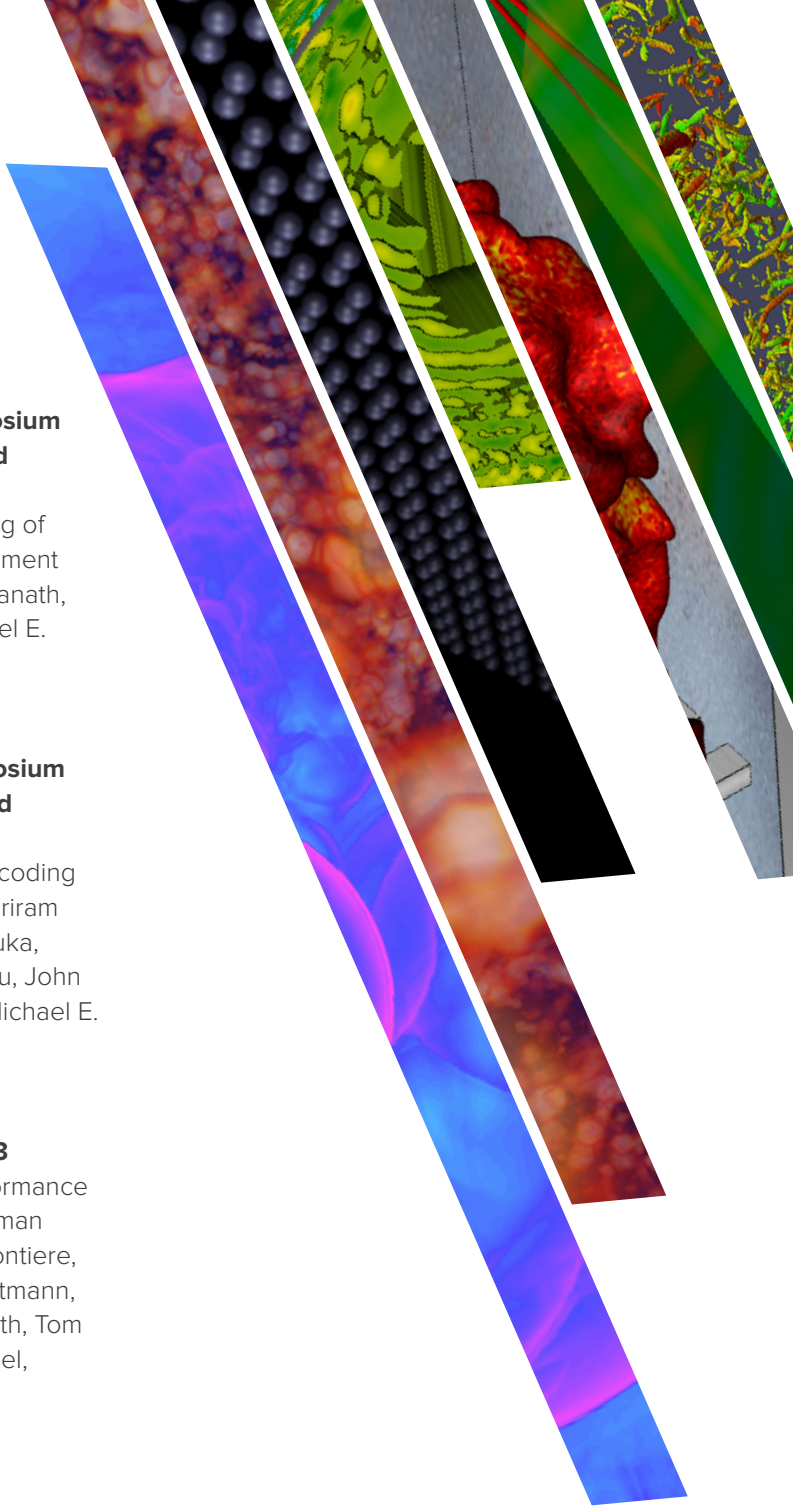
**Best Paper Award at IEEE Symposium on Large-Scale Data Analysis and Visualization**
"Efficient Parallel Volume Rendering of Large-Scale Adaptive Mesh Refinement Data." Nick Leaf, Venkatram Vishwanath, Joseph Insley, Mark Hereld, Michael E. Papka, Kwan-Liu Ma.

**Best Paper Award at ACM Symposium on High-Performance Parallel and Distributed Computing**
"Scalable In Situ Scientific Data Encoding for Analytical Query Processing." Sriram Lakshminarasimhan, David A. Boyuka, Saurabh V. Pendse, Xiaocheng Zou, John Jenkins, Venkatram Vishwanath, Michael E. Papka, Nagiza F. Samatova.

**Gordon Bell Prize Finalist at SC13**
"HACC: Extreme Scaling and Performance Across Diverse Architectures." Salman Habib, Vitali Morozov, Nicholas Frontiere, Hal Finkel, Adrian Pope, Katrin Heitmann, Kalyan Kumaran, Venkat Vishwanath, Tom Peterka, Joseph Insley, David Daniel, Patricia Fasel, Zarija Lukic.

**TOP500 List**
Mira ranked as the fifth fastest supercomputer in June and November.

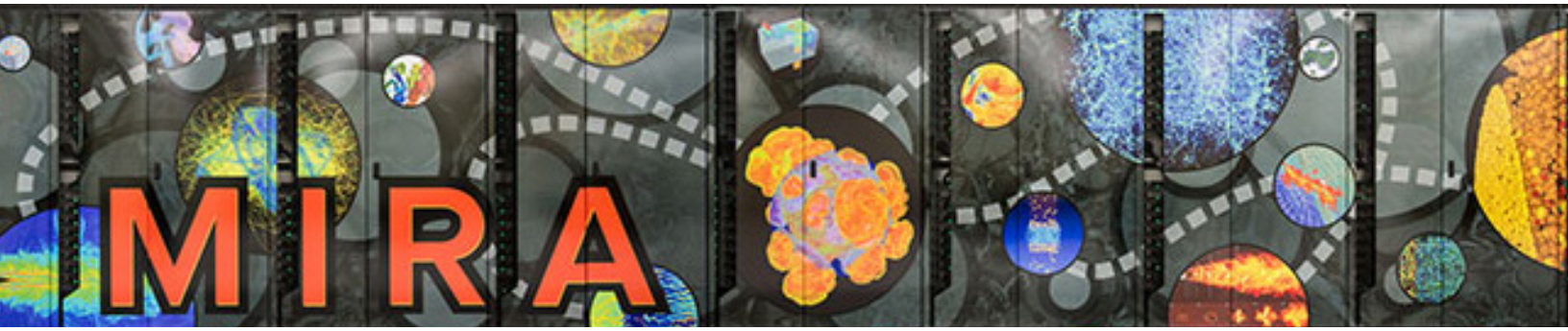
**Graph 500 List**
Mira ranked second using the Graph 500 benchmark in June and November.



# BLUE GENE/Q SYSTEMS

## MIRA

Mira, the ALCF's IBM Blue Gene/Q supercomputer, is equipped with 786,432 cores, 768 TB of memory, and has a peak performance of 10 petaflops. Mira's 49,152 compute nodes have a PowerPC A2 1600 MHz processor containing 16 cores, each with four hardware threads, and 16 GB of DDR3 memory. A 17th core is available for system services. Mira's 5D torus interconnect configuration, with 2 GB/s chip-to-chip links, connects the nodes, enabling highly efficient communication by reducing the average number of hops and latency between compute nodes. The Blue Gene/Q system also features a quad FPU that can be used to execute scalar floating-point instructions, four-wide SIMD instructions, or two-wide complex arithmetic SIMD instructions. This quad FPU provides higher single thread performance for some applications.



## VESTA

Vesta is the ALCF's test and development platform, serving as a launching pad for researchers planning to use Mira. Vesta has the same architecture as Mira, but on a much smaller scale (two computer racks compared to Mira's 48 racks). This system enables researchers to debug and scale up codes for the Blue Gene/Q architecture in preparation for Mira. Vesta has two racks, 2,048 nodes, 32 TB RAM, 5D torus interconnect, 32 I/O nodes, and a peak performance of 419 teraflops.

## CETUS

The primary role of Cetus is to run small jobs in order to debug problems that occur on Mira. It shares the same software environment and file systems as Mira. Cetus has one rack, 1,024 nodes, 32 TB RAM, 5D torus interconnect, eight I/O nodes, and a peak performance of 210 teraflops.

## TUKEY

Tukey is the analysis and visualization cluster for the ALCF's Blue Gene/Q systems. Equipped with state-of-the-art graphics processing units (GPUs), Tukey converts computational data from Mira into high-resolution visual representations. The resulting images, videos, and animations help users to better analyze and understand the data generated by Mira. Tukey can also be used for statistical analysis, helping to pinpoint trends in the simulation data. Additionally, the system is capable of preprocessing efforts, such as meshing, to assist users preparing for Mira simulations. Tukey shares the Mira network and parallel file system, enabling direct access to Mira-generated results. Each Tukey node has two 2 GHz 8-core AMD Opteron CPUs, two NVIDIA Tesla M2070 GPUs, and 64 GB of RAM. The full system has 96 nodes, 1,536 cores, a QDR InfiniBand interconnect, 6 TB of RAM, 1.1 TB of GPU RAM, and a GPU peak performance (aggregate) of over 99 teraflops (double precision).

# DATA STORAGE

The ALCF's data storage system is used to retain the data generated by simulations and visualizations. Disk storage provides intermediate-term storage for active projects, offering a means to access, analyze, and share simulation results. Tape storage is used to archive data from completed projects.

Disk Storage: The Blue Gene/Q data systems consist of 384 I/O nodes that connect to 16 storage area networks (SANs) that control 8,960 disk drives with a total capacity of 26.9 PB of raw storage and a maximum aggregate transfer speed of 240 GB/s. The ALCF uses the GPFS file system to access the storage.

Tape Storage: The ALCF's Blue Gene/Q and Blue Gene/P supercomputers share two 10,000-slot libraries using LTO4 tape technology. The LTO tape drives have built-in hardware compression with compression ratios typically between 1.25:1 and 2:1, depending on the data, giving an effective capacity of 16-24 PB.

# NETWORKING

Networking is the fabric that ties all of the ALCF's computing systems together. The Blue Gene/Q systems have an internal proprietary 5D torus network for communicating between nodes. InfiniBand enables communication between the I/O nodes and the storage system. Ethernet is used for external user access, and for maintenance and management of the systems.

The ALCF's Blue Gene/Q systems connect to other research institutions using a total of 100 Gb/s of external network connectivity. Scientists can transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and Internet2.

# BLUE GENE/P SYSTEMS

## INTREPID

Intrepid, the ALCF's IBM Blue Gene/P supercomputer, consists of 40 racks, 163,840 cores, 40,960 nodes, 80 TB of RAM, and has a peak performance of 557 teraflops. The system has a highly scalable 3D torus network, as well as a high-performance collective network that minimizes the bottlenecks common in simulations on large, parallel computers.

## CHALLENGER

Challenger is the home for the production and development job submission queue. It is intended for small, short, interactive debugging and test runs. Challenger has 4,096 cores, 1,024 nodes, 2 TB RAM and a peak performance of 13.9 teraflops.

## SURVEYOR

Surveyor is a Blue Gene/P system dedicated to tool and application porting, software testing and optimization, and systems software development. Surveyor has 4,096 cores, 1,024 nodes, 2 TB RAM, and a peak performance of 13.9 teraflops.

## EUREKA

Eureka is the ALCF's visualization and data analytics solution for the Blue Gene/P systems. Researchers use Eureka, a large installation of NVIDIA Quadro Plex S4 external GPUs, to facilitate data analytics and visualizations. By using the NVIDIA visual computing system as the base graphics building block, Eureka enables breakthrough levels of productivity and capability in visualization and data analysis. Eureka has 100 dual quad-core servers, 200 Quadro FX5600 GPUs, more than 3.2 TB of RAM, and a peak performance of 100 teraflops (single precision).

## GADZOOKS

Gadzooks test and development system for visualization. It has four compute nodes, each with two 2.0 GHz quad-core Xeon servers with 32 GB RAM, and eight NVIDIA Quadro FX5600 GPUs in two S4s.

## DATA STORAGE

The ALCF's data storage system is used to retain the data generated by simulations and visualizations. Disk storage provides intermediate-term storage for active projects, offering a means to access, analyze, and share simulation results. Tape storage is used to archive data from completed projects.

Disk Storage: The Blue Gene/P data systems consist of 640 I/O nodes that connect to 16 SANs that control 7,680 disk drives with a total capacity of 7.6 PB of raw storage and a maximum aggregate transfer speed of 88 GB/s. The ALCF uses two parallel file systems — PVFS and GPFS — to access the storage.

Tape Storage: The ALCF's Blue Gene/Q and Blue Gene/P supercomputers share two 10,000-slot libraries using LTO4 tape technology. The LTO tape drives have built-in hardware compression with compression ratios typically between 1.25:1 and 2:1, depending on the data, giving an effective capacity of 16-24 PB.

## NETWORKING

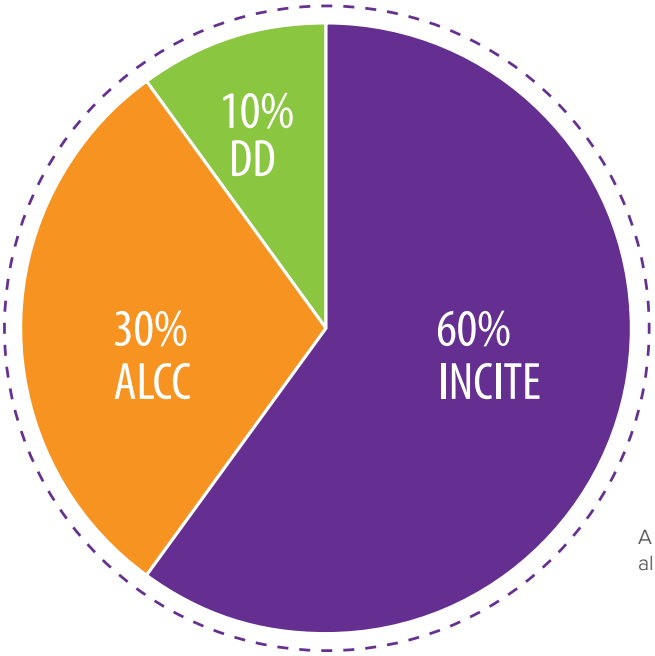
The ALCF's Blue Gene/P systems connect to other research institutions using a total of 20 Gb/s of external network connectivity. This allows scientists to transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and the Metropolitan Research and Education Network (MREN).

# **ALLOCATION** PROGRAMS

Any researcher with a question that requires large-scale computing systems can submit a proposal for time on ALCF resources to run simulations for their experiments. Typically awarded in chunks of millions of core-hours, the following allocation programs add up to billions of hours of computing time per year.

## INNOVATIVE & NOVEL COMPUTATIONAL IMPACT ON THEORY AND EXPERIMENT (INCITE)

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




A breakdown of how ALCF computing time is allotted among the three allocation programs.

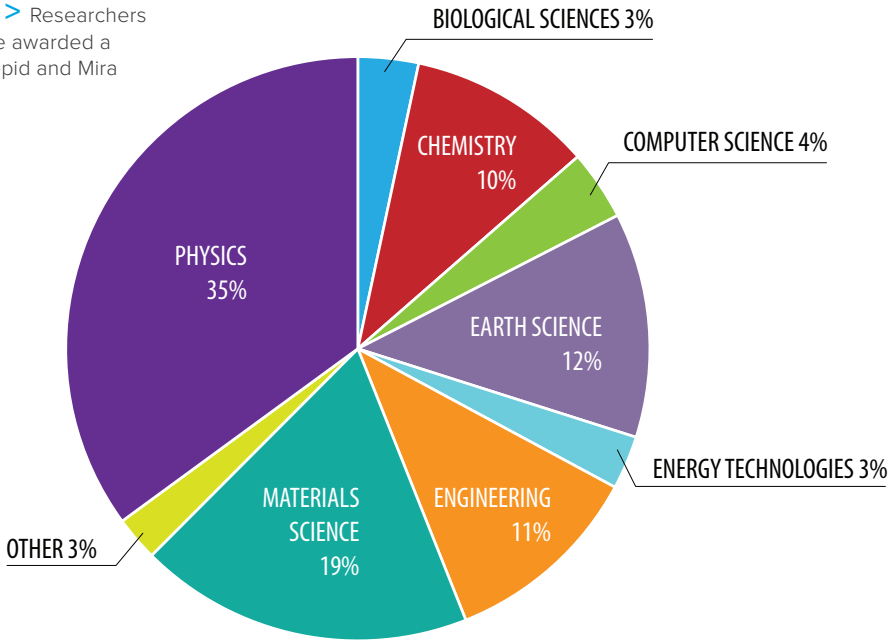
## ASCR LEADERSHIP COMPUTING CHALLENGE (ALCC)

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

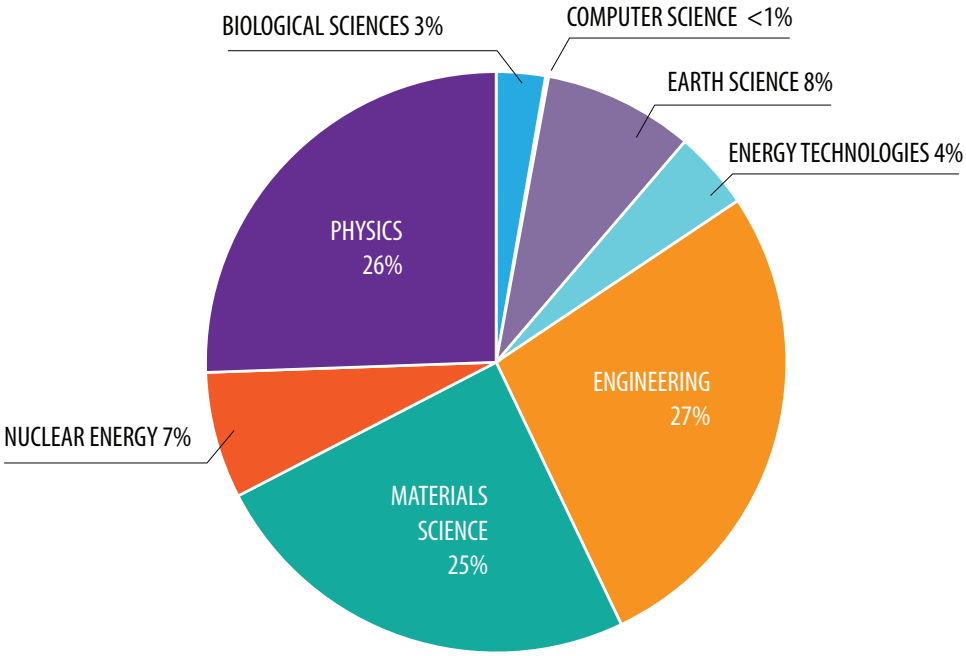
## DIRECTOR'S DISCRETIONARY (DD)

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

**2013 INCITE by Domain >** Researchers from a wide range of disciplines were awarded a total of 2.8 billion core-hours on Intrepid and Mira through the INCITE program in 2013.




**2013 by ALCC Domain >** Researchers pursuing DOE mission-related projects were awarded a total of 1.7 billion core-hours on Intrepid and Mira through the ALCC program in 2013.



# SCIENCE HIGHLIGHTS

**PI:** Juan de Pablo | depablo@uchicago.edu

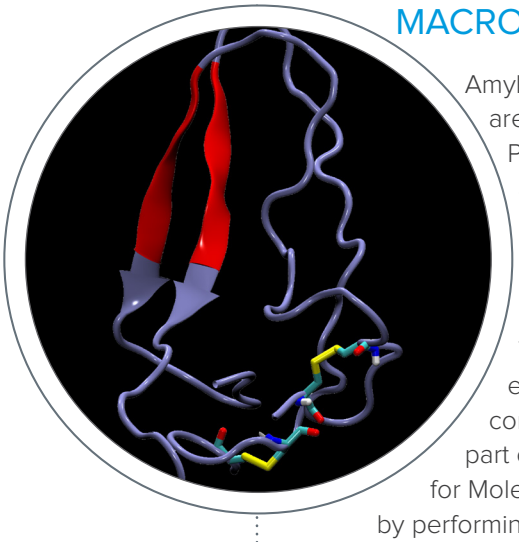
**INSTITUTION:** The University of Chicago

**ALLOCATION PROGRAM:** Director's Discretionary

**ALLOCATION HOURS:** 2 Million Core-Hours

**RESEARCH DOMAIN:** Biological Sciences

## MACROMOLECULAR FOLDING AND AGGREGATION



Amyloid fibrils are rod-shaped assemblies of misfolded proteins that are strongly associated with various diseases, including Alzheimer's, Parkinson's, and type 2 diabetes. These structures are believed to arise when proteins deviate from their normal 3D structures and instead adopt misfolded states that tend to clump. Understanding how amyloid fibrils develop is critical to controlling these tissue-damaging structures and developing new therapeutic strategies.

To investigate this issue, a multi-institutional team combined experimental and computational research efforts to uncover a complete picture of the early events leading to amyloid formation. As part of the research, scientists from the University of Chicago's Institute for Molecular Engineering interpreted experimental spectroscopic data by performing large-scale molecular simulations with with Intrepid at the ALCF and computing resources at the University of Chicago. The results supplied an essential model of the molecular steps involved in the reaction.

The research team located an entire step that had been missing, and whose absence had been fueling confusion. An earlier study indicated that the intermediate step was likely a floppy loop area formed by proteins, which did not seem compatible with the tough, damaging fibril as an end result. Researchers believed that the fibrils should come from a rigid structure called a β-sheet. The new data show, however, that both structures occur as the reaction changes over time. Transient rigid β-sheets form, then morph into floppy protein loops, which finally take the form of more β-sheets. The final β-sheets bind together and stack up to form the damaging fibrils.

The researchers will continue to investigate amyloid fibrils at the ALCF as part of a 2014 INCITE allocation. With more data, the research could lead to the design of an inhibitor drug to bind to the offending protein, block the molecule, and halt the pathway's progression.

Representative configuration from the transition state ensemble of two amylin molecules forming a dimer. The red-colored regions correspond to a β-sheet .

*Image Credit: Chi-Cheng Chiu, Argonne National Laboratory/ The University of Chicago*

**IMPACT »** This work helped pinpoint a critical intermediate step in the chemical pathway involved in the development of amyloid fibrils. Future work could target a possible treatment, such as designing an inhibitor to interfere with the harmful pathway.

**PI:** Benoît Roux | roux@uchicago.edu

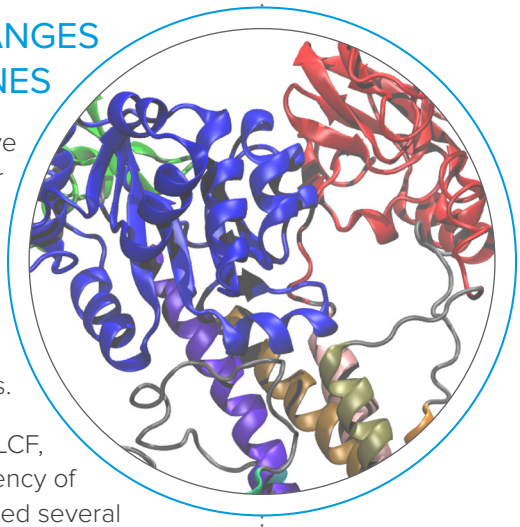
**INSTITUTION:** The University of Chicago

**ALLOCATION PROGRAM:** INCITE/ESP

**ALLOCATION HOURS:** 55 Million/80 Million Core-Hours

**RESEARCH DOMAIN:** Biological Sciences

# STUDIES OF LARGE CONFORMATIONAL CHANGES IN BIOMOLECULAR MACHINES



Molecular dynamics (MD) simulations provide a new perspective to understand the function of biologically important molecular systems. The success of MD simulations are determined by the accuracy of the potential function and on the efficiency of the dynamic algorithm enabling the adequate sampling of motions. NAMD, a high-performance code under development at the University of Illinois, is one of the most optimal programs used to carry out classical simulations of biomolecular systems.

Through an Early Science Program (ESP) project at the ALCF, University of Chicago researchers enhanced the sampling efficiency of NAMD beyond that of brute-force MD simulations, and implemented several advanced strategies based on multiple copies such as temperature and Hamiltonian tempering replica-exchange MD (T-REMD and H-REMD). They also implemented a new force field that incorporates the effect of induced polarization.

To further research using NAMD, the research team used a 2013 INCITE award to conduct simulations to gain a deep mechanistic perspective of protein function, linking structure to dynamics by characterizing the free energy landscape that governs key functional motions. In the case of the c-Src tyrosine kinase, researchers studied the effects of its regulatory domains on the activation transition using the swarms-of-trajectories method and confirmed by potential of mean force calculations. Large domain motions were also studied in the ATP-driven ion pumps, where the first leg of the catalytic cycle has been characterized.

Cytoplasmic domains of the ATP-driven calcium pump SERCA.

*Image Credit: Avisek Das, The University of Chicago*

**IMPACT »** The enhancements made to NAMD through this project have provided an investigative tool of unprecedented accuracy for the entire scientific community, enabling studies of biological systems that were not possible in the past. Results from the INCITE project will serve as a roadmap for simulating, visualizing, and elucidating how biomolecular nano-machines work.

**PI:** Thierry Poinsot | poinsot@cerfacs.fr

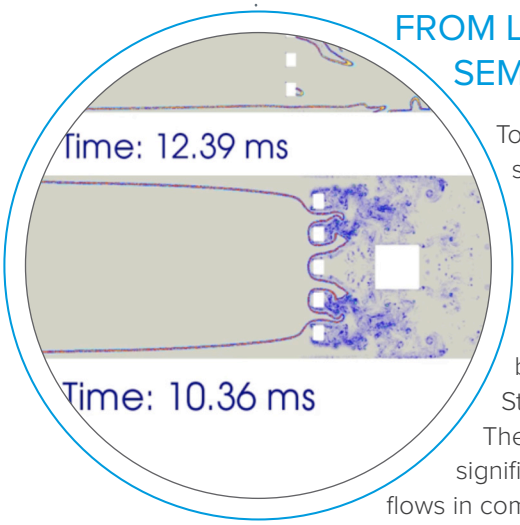
**INSTITUTION:** CERFACS

**ALLOCATION PROGRAM:** INCITE

**ALLOCATION HOURS:** 20 Million Core-Hours

**RESEARCH DOMAIN:** Chemistry

## FROM LES TO DNS OF EXPLOSIONS IN SEMI-CONFINED DOMAINS




To aid in the design of safer buildings, researchers often use simulations to evaluate the potential impacts of explosions caused by gas leaks. This is especially critical in the oil industry, where leaks are common. Such accidents can lead to a financial loss, and more devastatingly, a loss of lives.

Traditionally, safety-related studies of explosions for industry have been carried out using Unsteady Reynolds Averaged Navier-Stokes (URANS) methods, which rely on crude parametrizations. The recent emergence of large eddy simulations (LES) has significantly improved the ability to precisely simulate fully unsteady flows in complex geometries with much less parametrization and uncertainty. In small-scale devices, even direct numerical simulations are feasible today.

For this INCITE project, researchers at CERFACS set out to develop high-fidelity LES tools for realistic explosion cases, with sizes on the order of 10 to 100 m and very large Reynolds numbers. To ensure they captured all phases of the flame development, the research team began with a smaller experimental setup (25 cm) for LES validation. Using Mira they were able to perform the first simulation of an explosion in a building on a one-billion-cell mesh. The comparison between the simulation and experimental results, obtained without ad-hoc parametrization, proved to be very good.

Due to the project's success, the experimental setup for the LES validation has been replicated in Norway (GexCon) at two new scales (6 and 24 times larger). This created a unique experimental database where scaling laws can be tested on a range that has never been seen in the turbulent combustion community, opening the door to new LES research into explosions and turbulent premixed combustion modeling in general.

Flame position and turbulent viscosity at two instants after ignition took place on the left side of the building.

*Image Credit: Thierry Poinsot, CERFACS*

**IMPACT »** A better understanding of the mechanisms controlling explosions in confined spaces will lead to the design of safer buildings. This project has also driven new experiments that are helping to expand the scope of turbulent combustion research.

**PI:** Hal Finkel | hfinkel@anl.gov

**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** Director's Discretionary

**ALLOCATION HOURS:** 50,000 Core-Hours

**RESEARCH DOMAIN:** Computer Science

## OPEN SOURCE COMPILING FOR SUPERCOMPUTERS

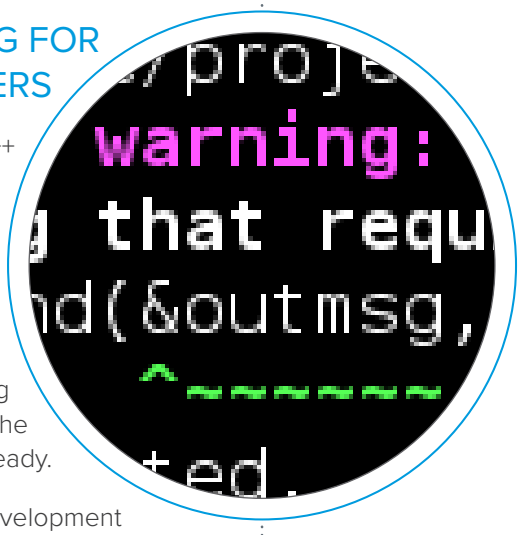
In 2013, the ALCF continued the development of the bgclang C/C++ compiler for its IBM Blue Gene/Q systems. This compiler is derived from the open-source LLVM/Clang compiler, which is jointly developed by Apple, Google, Intel, ARM, AMD, Nvidia, IBM, and a number of other companies, research groups, and individuals. Unlike the closed-source or open-source (but unoptimized) compilers provided for Blue Gene systems, the bgclang compiler supports the latest language standards (e.g., C++11) while being optimized for Blue Gene. There is more work to be done, but the bgclang compiler is now production ready.

The ALCF's in-house experts have had a direct impact on the development of the compiler features. A large fraction of the improvements to LLVM and Clang developed as part of this project have been contributed to the LLVM/Clang upstream codebase for the benefit of all LLVM/Clang users. With assistance from IBM, ALCF maintains the LLVM PowerPC backend. The development of bgclang directly benefits the ALCF community by allowing users to access a development framework on Blue Gene/Q systems that is very similar to the environment available on their laptops. The effort has also helped raise the profile of ALCF within the compiler community and fostered a closer relationship with vendors.

Already, bgclang has enabled the running of vectorized C++11 applications on the ALCF's IBM Blue Gene/Q resources, a feat impossible with the vendor-supplied toolchains. In addition, the MPI-specific warning messages and instrumentation-based memory debugging facilities have been used to find bugs in several applications, including HACC. (Hardware/Hybrid Accelerated Cosmology Code)

The bgclang compiler, including associated MPI wrapper scripts, is installed and documented on all of the ALCF's Blue Gene/Q systems. The project page also contains the binary and source downloadable archives for use on Blue Gene/Q systems elsewhere. The tool is currently being used at several Blue Gene/Q sites outside of Argonne, including Lawrence Livermore National Laboratory.

**IMPACT »** The ALCF-developed bgclang C/C++ compiler provides a tool to enable easier code development, porting, and performance. It also gives the leadership-computing community an open source, optimizing compiler that supports the same modern C++ programming language available on their laptops.




MPI-specific warning messages like this were first made available to ALCF users, but are now available upstream in both Clang and MPICH.

*Image Credit: Hal Finkel, Argonne National Laboratory*

**PI:** Michael E. Papka | papka@anl.gov

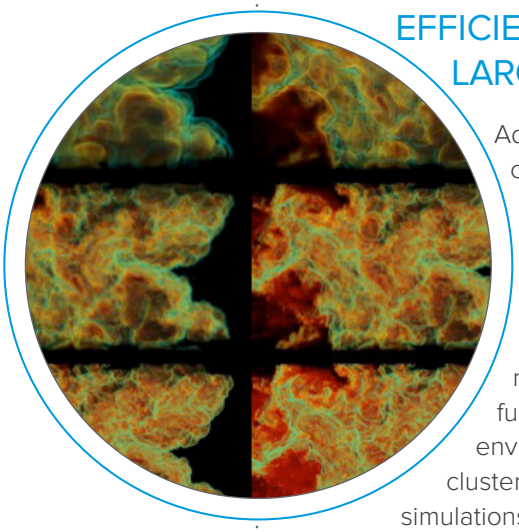
**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** Director's Discretionary

**ALLOCATION HOURS:** 125,000 Core-Hours

**RESEARCH DOMAIN:** Computer Science

## EFFICIENT PARALLEL VOLUME RENDERING OF LARGE-SCALE ADAPTIVE MESH REFINEMENT DATA



This image shows the progressive refinement of a Rayleigh-Taylor flame using a parallel visualization method for AMR simulation data. The variable being visualized is an analytical estimate of the flame front. The green-blue color highlights the flame surface, and the yellow-orange-red transition shows the fuel-ash mixture, which the flame front leaves behind.

*Image Credit: Carlo Graziani and Don Lamb, The University of Chicago*

Adaptive mesh refinement (AMR) is a popular method used by computational scientists to allocate scarce computing resources to the most important portions of the simulation domain during the time the solution is being calculated. Visualization of large-scale AMR data is of great interest to this community, and interactivity is a critical part of visualization's usefulness as an exploration tool. The complexity of AMR requires correct interpolation between refinement levels for high-quality images. Technical challenges are further compounded by the complex and heterogeneous computing environment, which must be multi-way parallel (both in the GPU and cluster sense) in order to cope with the large data sizes of modern AMR simulations.

For this joint project, researchers from Argonne National Laboratory, the University of California, Davis, and the FLASH Center for Computational Science at the University of Chicago collaborated to develop a parallel visualization method for AMR. The team used the existing AMR structure to subdivide the problem into convexly bounded chunks and perform static load balancing. They took advantage of data locality within chunks to interpolate directly between blocks without the need to store ghost cells on the interior boundaries. The researchers developed a novel block decomposition method and analyzed its performance against two alternative methods. The comparison of the block decomposition methods found that the per-region decomposition yielded the fastest rendering time unless the choice of view produced a large number of sub-pixel blocks. Additionally, the research team illustrated the scalability of the renderer using weak and strong scaling measurements and showed that it scales in line with comparable renderers for regular grid volume rendering. The project resulted in a paper that won the Best Paper Award at the IEEE Symposium on Large Data Analysis and Visualization in October 2013.

**IMPACT »** Computational science simulations running on DOE leadership computing systems are increasingly adopting AMR. The Argonne team's parallel visualization method will be key to gleaning insights from the large-scale datasets generated by AMR simulations. This type of scalable mechanism to visualize AMR simulations becomes increasingly important as the amount of data generated with future systems continues to grow.

**PI:** Michael Crowley | michael.crowley@nrel.gov

**INSTITUTION:** National Renewable Energy Laboratory

**ALLOCATION PROGRAM:** INCITE

**ALLOCATION HOURS:** 70 Million Core-Hours

**RESEARCH DOMAIN:** Energy Technologies

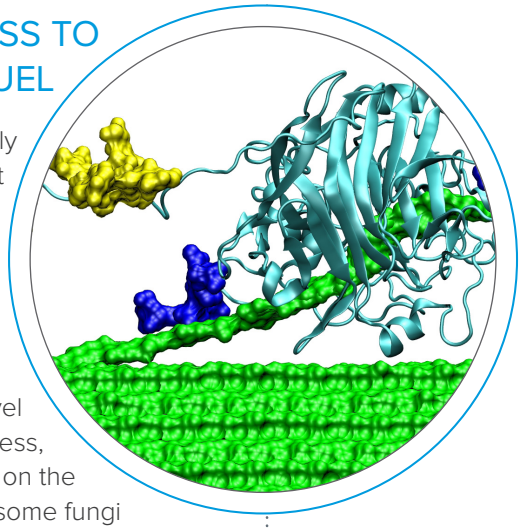
# THERMODYNAMICS OF BINDING BIOMASS TO CELLULASES FOR RENEWABLE FUEL

Biofuel feedstocks, such as wood chips and switchgrass, naturally resist being broken down into fermentable sugars, making it difficult to produce biofuels at a cost and pace that can compete with fossil fuels. For this INCITE project, researchers used ALCF supercomputers to study nature's catalysts, enzymes, for inspiration in their quest to find a more effective means of converting biomass into renewable fuel.

The research team carried out simulations to gain a molecular-level understanding of the complex cellulose-to-sugar conversion process, known as enzymatic hydrolysis. Their simulation efforts focused on the physical behavior of cellulase enzymes. Naturally produced by some fungi and bacteria, these particular enzymes were selected for modeling because they effectively trigger the chemical changes necessary to degrade hardy plant materials into life-sustaining sugars.

Using Intrepid and Mira, the researchers ran large-scale free energy perturbation simulations of the enzymes. Supplemented by additional calculations performed through National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) program, they were able to obtain accurate binding free energy information for several model enzymes relevant to biofuels production.

The binding free energy values suggest saccharide morphology is susceptible to enzyme action. Additionally, the research shows that ligand binding free energy is a key parameter in comparing the activity and function of enzymes. This information can help inform improved experimental design approaches to develop superior enzymes and less recalcitrant plant-based feedstocks for liquid biofuels.



An enzyme from the fungus *Trichoderma reesei* is shown digesting cellulose (green). The enzyme consists of three sub-domains: a small carbohydrate-binding module; a long, flexible linker decorated with *O*-linked glycosylation (yellow); and a large catalytic domain (CD) with N-linked glycosylation (blue); and a 50 Å tunnel for the threading of cellodextrin for catalytic cleavage.

*Image Credit: Gregg Beckham, National Renewable Energy Laboratory*

**IMPACT »** The project addresses a national goal to make biofuels a more prevalent and reliable option as an alternative transportation fuel. With a better understanding of enzyme behavior, researchers can identify potential enzyme modifications and then feed those discoveries into experiments to develop and validate improved biofuel catalysts.

**PI:** Robert Moser | rmoser@ices.utexas.edu

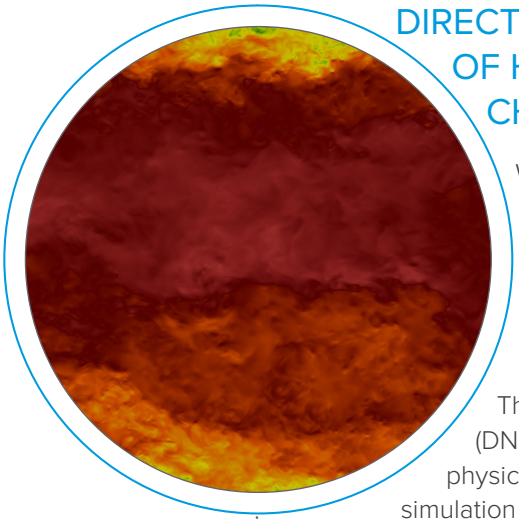
**INSTITUTION:** University of Texas at Austin

**ALLOCATION PROGRAM:** INCITE/ESP

**ALLOCATION HOURS:** 175 Million/60 Million Core-Hours

**RESEARCH DOMAIN:** Engineering

# DIRECT NUMERICAL SIMULATIONS OF HIGH REYNOLDS NUMBER TURBULENT CHANNEL FLOW



Wall-bounded turbulence is at the heart of the interaction between solid surfaces (such as vehicles and pipes) and the fluid flowing past them, leading to drag and the dissipation of energy. Engineering developments to reduce drag and energy consumption are greatly impeded by the lack of accurate models of the turbulence phenomena involved.

The goal of this project was to perform direct numerical simulations (DNS) of high Reynolds number fluid flow to examine the complex physics of wall-bounded turbulence. The subsequent analysis of the simulation data can provide the insights needed to develop improved turbulence models, as well as new concepts for manipulating wall-bounded turbulence.

The research team was particularly interested in the overlap region, where the viscous near-wall turbulence interacts with the outer-layer turbulences. This region is currently not well understood because simulations to date have not allowed for a sufficiently high Reynolds number to obtain the scale separation needed to shed light on the complexity of this multiscale turbulent structure. However, with the computational power of Mira, this project was able to run DNS with a high enough Reynolds number to generate sufficient scale separation. Given the mesh size (15360 x 1536 x 11520), the simulations are believed to be the largest production DNS ever performed. Prior to this research, the standard reference data set for turbulence research covered the friction-Reynolds-number range $Re_\tau = 180–2000$. Supplementing these data with $Re_\tau = 5200$ from the simulations on Mira will establish a reference dataset that will remain useful for the turbulence research community for many years to come.

This visualization depicts the instantaneous streamwise velocity component over a section of streamwise length of the simulated channel. The image is from a simulation of incompressible turbulent flow ($Re_\tau = 5200$) between two parallel smooth planes.

*Image Credit: Nicholas Malaya, University of Texas at Austin*

**IMPACT »** Results from this project will provide insights necessary to develop more accurate turbulence models. Ultimately, this work could lead to more energy-efficient transportation through the design of improved vehicle surfaces and reduced-drag piping and ducts.

**PI:** Umesh Paliath | paliath@ge.com

**INSTITUTION:** GE Global Research

**ALLOCATION PROGRAM:** INCITE

**ALLOCATION HOURS:** 105 Million Core-Hours

**RESEARCH DOMAIN:** Engineering

# ENABLING GREEN ENERGY AND PROPULSION SYSTEMS VIA DIRECT NOISE COMPUTATION

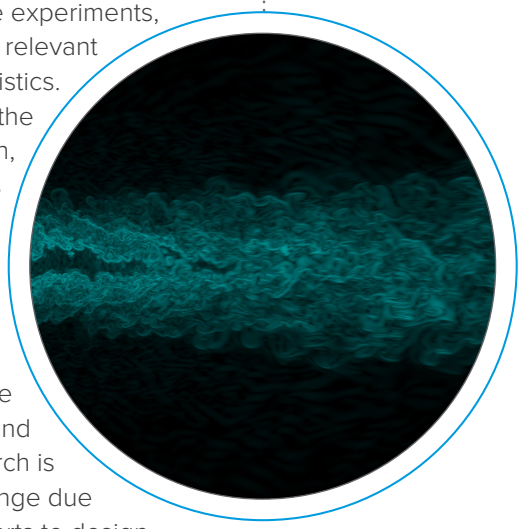
**High-performance computing at the ALCF is enabling a team from GE Global Research to understand and visualize the complex phenomena of turbulent mixing in jet exhaust flow and flow over wind turbine airfoils in ways not possible in experiments**

## Decreasing Jet Engine Noise

Understanding the complex turbulent mixing noise sources for jet exhaust nozzles is critical to developing effective noise-control strategies for a new generation of more efficient and environmentally friendly aircraft engines.

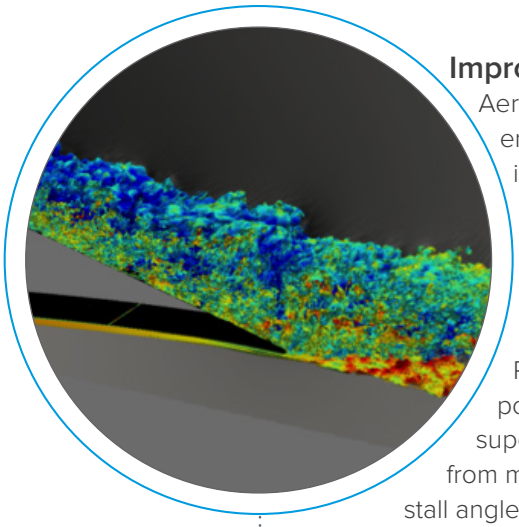
GE Global Research has developed large eddy simulation (LES) methodology to break barriers in accurately characterizing the key flow physics of multiscale turbulent mixing in boundary layer and free shear flows. The approach is enabling GE to predict the acoustic signature from complex exhaust nozzles with noise-control devices such as chevrons and lobed mixers.

GE researchers are using the LES method as a numerical wind tunnel to provide insight into noise generation and radiation mechanisms. Unlike experiments, the virtual wind tunnel allows for simultaneous measurement of all relevant turbulent quantities to reconstruct higher-order turbulence statistics. The resulting datasets will be used to evaluate and improve the current assumptions in reduced-order acoustic models. In addition, using modal analysis as a post-processing tool, the researchers can shed light on the effect the exhaust nozzle shape has on noise generation and propagation. With a filtered Proper Orthogonal Decomposition code, the team used the time-accurate data gathered from the virtual wind tunnel to evaluate the sound radiating flow modes of a jet. This approach is being applied to a baseline conic nozzle and three chevron nozzle configurations. The number of modes that actually propagate sound were identified to be a small fraction of the flow modes. Research is in progress to understand how these noise-radiating modes change due to nozzle geometry variation. This will be extremely useful in efforts to design quieter and more efficient exhaust nozzles.



Noise generation due to turbulent mixing of exhaust flow. Large eddy simulation of exhaust flow from a two-inch conic nozzle with exit Mach number of 0.97. Visualizing density gradients in the flow.

*Image Credit: Joseph Insley, Argonne National Laboratory; Umesh Paliath, GE Global Research*



Separated flow near the trailing edge of a wind turbine airfoil. Results from a large eddy simulation of the DU96-W180 airfoil at Reynolds number of 1.5 million and flow angle of 10.3°. Flow separating from the airfoil visualized by Q-criterion iso-surfaces colored by the vertical velocity.

*Image Credit: Joseph Insley, Argonne National Laboratory; Lawrence Cheung, Giridhar Jothiprasad, Swati Saxena, Prem Venugopal, GE Global Research*

## Improving Wind Turbine Design

Aerodynamic noise and loads control are key barriers to enhancing energy yield from wind turbines. As the size of wind turbines increases and cost-reduction targets encourage lighter, more flexible structures, the ability to accurately predict and design for the impact of these factors has become increasingly important.

LES through direct computation of flow separation and noise sources provides greater predictive potential than traditional Reynolds-Averaged Navier Stokes (RANS) methods. For this portion of the INCITE allocation, the GE research team used ALCF supercomputers to expand the envelope of LES airfoil predictions from moderate- to lab-scale Reynolds numbers (1.5 million) and to near-stall angles with significant separation regions. For a representative wind turbine airfoil in attached flow, both aerodynamics and far-field noise predictions agreed favorably with experimental data. Following which, LES simulations were planned at near-stall flow incidences with separated flow.

The GE team collected data to assess the capability of LES to accurately capture the reduced lift near-stall that is missed by other engineering tools such as RANS models. The LES calculations for the DU96 airfoil (a representative wind turbine airfoil profile) at an angle of attack of 10.3° and a Reynolds number of 1.5 million are complete, and flow statistics have been collected over two chord flow-through times. The LES data will help further the understanding of flow physics in separated regions on the airfoil. Key flow parameters such as overall lift, transition, and flow separation locations on the airfoil surface are being post processed from these simulations.

While near-stall conditions are particularly challenging for flow solvers due to flow separation over significant portions of the airfoil, preliminary results from a near-stall LES performed at the ALCF show encouraging signs of reduced lift. LES datasets collected for this project will improve the understanding of separated flow physics and provide hard-to-measure statistics for improving RANS-based CFD approaches.

**IMPACT »** Findings from this research will significantly improve the prediction and design capabilities for next-generation aircraft engines and wind turbines, both from demonstrating the viability of LES as a characterization tool and as a source of physics guidance.

**PI:** Subramanian Sankaranarayanan | ssankaranarayanan@anl.gov

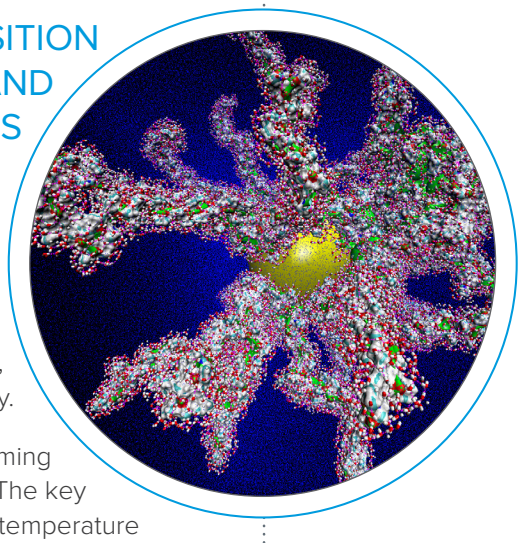
**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** ALCC

**ALLOCATION HOURS:** 50 Million Core-Hours

**RESEARCH DOMAIN:** Materials Science

# DYNAMICS OF CONFORMATIONAL TRANSITION IN THERMO-SENSITIVE POLYMERS AND HYDROGELS



Chemists have been studying polymers and gels for decades to see how these large chains of molecules respond to external stimuli such as heat, pH, temperature, electric fields, light, and chemical influences. Their goal is to find ways to control the polymers' actions and behaviors for a wide range of applications: drug delivery, medical diagnostics, tissue engineering, electrophoresis, and enhanced oil recovery.

Certain smart polymers, for instance, rely on heat, water, and timing to execute their missions in controlled drug delivery systems. The key to employing a polymer is controlling its lower critical solution temperature (LCST). When reached, the LCST triggers a dramatic conformational change in which the polymer chain goes from an expanded coil state to a collapsed, globular one. A model biopolymer, called thermosensitive poly(n-isopropylacrylamide) – PNIPAM or Poly NIPAM – has drawn considerable attention because its LCST nearly matches human body temperature, which is critical in drug delivery systems.

For this ALCC project, researchers studied how polymers respond to temperature, so that when the polymers are systematically heated and cooled across their LCST, the team could observe how their conformations change and respond to their environment, in particular water. The researchers ran simulations on Intrepid using molecular dynamics programs, LAMMPS and NAMD, to track the interactions of 32 million atoms at a time. The goal of these simulations was to understand the atomistic origin of the coil-to-globule phase transition in PNIPAM. The team's main finding was that the ordering of water molecules plays a critical role in dictating the polymer conformation. In particular, the surrounding water forms cage-like structures, which drive the coil-to-globule phase transition in PNIPAM. The researchers will continue their work on the smart polymers on Mira in 2014.

Atomistic simulations illustrate the influence of solvation dynamics on the conformation transition in a PNIPAM (poly(N-isopropyl-acryl-amide)) brush structure grafted on a gold nanoparticle.

*Image Credit: Sanket Deshmukh, Derrick Mancini, and Subramanian Sankaranarayanan, Argonne National Laboratory; Ganesh Kamath, University of Missouri*

**IMPACT »** As a result of this work, researchers developed a fundamental understanding of stimuli response of smart polymers and identified the role of solvation in inducing phase transition. Long term, this work could help improve the design of controlled drug delivery systems.

**PI:** Larry Curtiss | curtiss@anl.gov

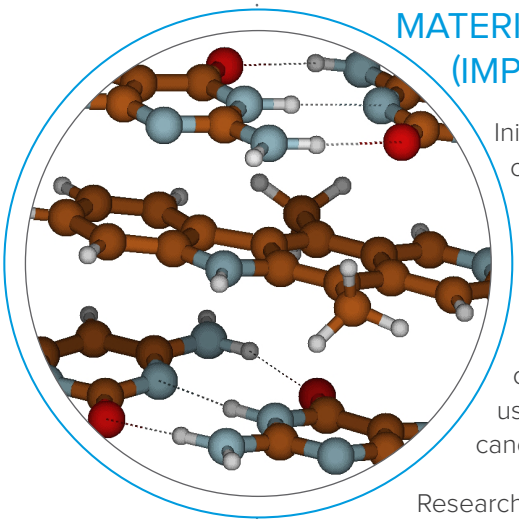
**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** ESP

**ALLOCATION HOURS:** 50 Million Core-Hours

**RESEARCH DOMAIN:** Materials Science

## MATERIALS DESIGN AND DISCOVERY (IMPROVING CANCER DRUG DESIGN)



Initially aimed at performing density functional theory calculations on materials for energy storage and catalysis, the research team shifted the focus of this Early Science Program project after determining intrinsic algorithmic limitations. Instead, Argonne researchers decided to pursue the optimization of Quantum Monte Carlo (QMC) as a complimentary method on Mira, providing a valuable tool for the scientific community. As part of their work, the team was able to demonstrate the potential of using QMC in their studies of ellipticine, a promising drug for uterine cancer treatment.

Research in drug action at the molecular level depends primarily on understanding and defining the physical/chemical interaction between the drug and its receptor, and then understanding how to connect this interaction to the pharmacological response. Over the past couple of decades, the screening of molecules for their active principle has relied greatly on the ability to model candidate molecules before experimental consideration. This task can only be achieved with an *ab initio* quantum chemistry theory, such as QMC, that takes electron correlation effects into account.

For their groundbreaking studies of ellipticine, the Argonne research team used the scalable QMCPACK simulation package. With Mira, the researchers were able to obtain a highly accurate binding energy calculation (at chemical accuracy of ~1 kcal/mol) of ellipticine to DNA (33.6 ±0.9 kcal/mol), while other traditional methods had predicted no binding (DFT: -5 kcal/mol). This case study shows the reliability and efficiency of QMC for characterizing the binding energies for biological systems, providing a critical input for improved drug modeling efforts.

Ellipticine is shown in the middle binding to the DNA of cancer cells.

*Image Credit: Anouar Benali, Argonne National Laboratory*

**IMPACT »** This research effort demonstrated the potential of using QMC methods on leadership-class supercomputers to accelerate the design and development of promising new drugs, such as ellipticine. The project also proved that many molecules thought to be too complicated for quantum chemistry could be tackled by QMC methods.

**PI:** Priya Vashishta | priyav@usc.edu

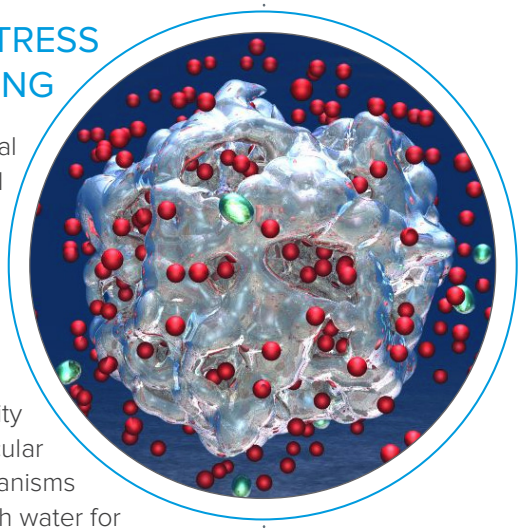
**INSTITUTION:** University of Southern California

**ALLOCATION PROGRAM:** INCITE

**ALLOCATION HOURS:** 240 Million Core-Hours

**RESEARCH DOMAIN:** Materials Science

# PETASCALE SIMULATIONS OF STRESS CORROSION CRACKING



Producing hydrogen from aluminum-water reactions has potential for many clean energy applications, including on-board fuel production for hydrogen-powered vehicles. The approach has been limited by scalability issues due to poor yields using aluminum particles, but recent experiments have suggested that alloying aluminum with lithium could enhance the reaction rate and achieve 100% yield for hydrogen production.

In the final year of this three-year INCITE allocation, University of Southern California researchers performed quantum molecular dynamics (QMD) simulations on Mira to study the atomistic mechanisms of the reaction of a lithium-aluminum (Li-Al) alloy particle with water for on-demand hydrogen gas production. The research team previously used the allocation to investigate fundamental mechanisms of stress corrosion cracking, nanoindentation of amorphous silica in the presence of water, and impurity segregation-induced embrittlement of metallic alloys.

For the hydrogen production study, the researchers completed a 16,611-atom QMD simulation to analyze the reaction that leads to rapid, high-yield hydrogen production. The simulations revealed that alloying Al particles with Li results in orders-of-magnitude acceleration of the reaction rate as well as higher yield. The key atomistic mechanisms that were identified include efficient charge pathways in Al atoms that collectively act as a "superanion" and dissolution of Li atoms into water that produces a corrosive basic solution to prevent the formation of a passive oxide layer on the particle surface.

To investigate the problem of scalability, the researchers compared simulations involving $Li_{135}Al_{135}$ and $Li_{441}Al_{441}$ in water (total of 4,836 and 16,611 atoms, respectively). They found the $Li_nAl_n$ surface is equally reactive regardless of the surface curvature, indicating the alloy design has the potential to scale up to industrially relevant particle sizes.

**IMPACT »** These simulations provide a microscopic understanding of how hydrogen is produced from water reacting with lithium-aluminum alloy nanoparticles, while validating its potential for industrial scalability. Results from this INCITE project can inform design principles for rapid, high-yield hydrogen production for clean energy applications such as hydrogen-powered vehicles.

Hydrogen production from water using a $Li_{441}Al_{441}$ particle. The valance electron density represented by the silver isosurface is centered around Al atoms, whereas some of the Li atoms represented by red spheres are dissolved into water. Produced hydrogen molecules are represented by green surfaces. Water molecules are not shown for the clarity of presentation.

*Image Credit: Rajiv Kalia, Aiichiro Nakano, Ken-ichi Nomura, and Priya Vashishta, University of Southern California; Kohei Shimamura and Fuyuki Shimojo, Kumamoto University, Japan*

**PI:** Robert A. DiStasio Jr. | distasio@princeton.edu

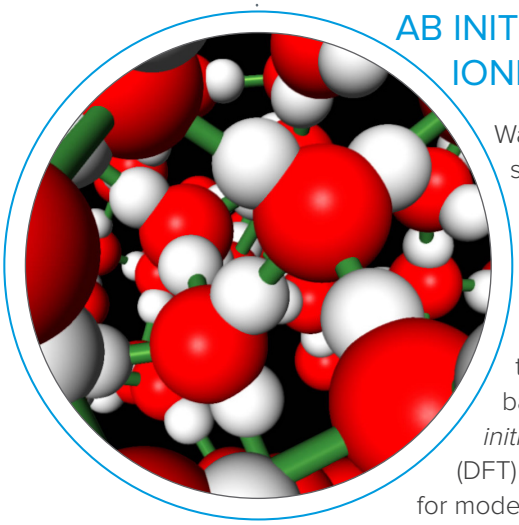
**INSTITUTION:** Princeton University

**ALLOCATION PROGRAM:** ALCC

**ALLOCATION HOURS:** 250 Million Core-Hours

**RESEARCH DOMAIN:** Physics

# AB INITIO QUANTUM LIQUID WATER AND AQUEOUS IONIC SOLUTIONS



Water is arguably the most important molecule on Earth. While a single water molecule has a simple and well-known structure, the unique physical and chemical properties of liquid water are largely due to the presence of complex networks of hydrogen bonds governing the interactions between individual water molecules.

At present, no experimental methodology exists to directly obtain the microscopic structure of liquid water; however, computer-based simulations can furnish such structural information. While *ab initio* molecular dynamics (AIMD) based on density functional theory (DFT) is the most accurate and widely used computational methodology for modeling condensed phase systems, this approach has severe limitations when applied to liquid water.

This ALCC project seeks to provide highly accurate benchmark atomistic simulations of liquid water by combining novel algorithmic and theoretical developments to address these limitations and extend the current state-of-the-art in computational molecular modeling. In addition, researchers are investigating a series of fundamental aqueous ionic solutions, starting with the hydronium ($H_3O^+$) and hydroxide ($OH^-$) ions (models of acidic and basic conditions), and continuing with the ions relevant to the design of novel clean energy materials, such as aqueous ion batteries.

These large-scale simulations, which can only be accomplished with high-performance massively parallel supercomputers like the ALCF's IBM Blue Gene/Q platform, are part of the "Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments" project funded by DOE's Scientific Discovery through Advanced Computing (SciDAC) program. This SciDAC project is a collaborative effort between Princeton University, Temple University, and Lawrence Berkeley National Laboratory.

Model of the microscopic structure of liquid water. Oxygen and hydrogen atoms are depicted by red and white spheres, respectively. The hydrogen bond network is represented by green tubes.

*Image Credit: F. W. Starr, Wesleyan University*

**IMPACT »** These benchmark simulations will provide detailed knowledge of the coordination shell structure and atomic pair correlation functions of liquid water and aqueous ionic solutions with unprecedented accuracy, and address important renewable energy research issues, in particular the understanding and rational design of aqueous ion batteries. The results will be stored in a publicly available structural database to serve as an invaluable resource for further theoretical investigations and developments.

**PI:** Steven Pieper | spieper@anl.gov

**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** ESP

**ALLOCATION HOURS:** 110 Million Core-Hours

**RESEARCH DOMAIN:** Physics

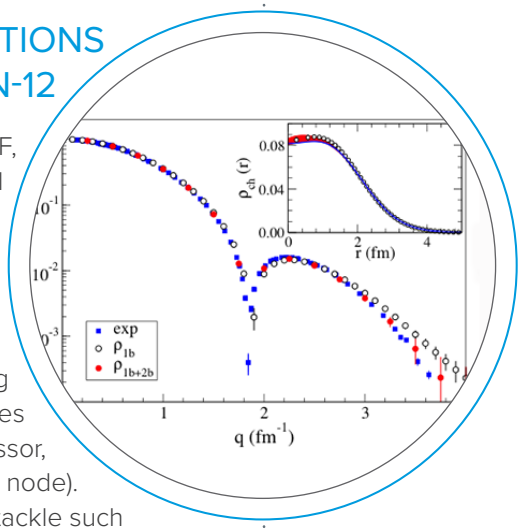
# AB INITIO REACTION CALCULATIONS FOR CARBON-12

With an Early Science Program (ESP) project at the ALCF, researchers from Argonne, Los Alamos, and Jefferson national laboratories used Mira to make reliable fundamental calculations of neutrino and electron reactions with carbon-12 nuclei.

The researchers tuned the Green's Function Monte Carlo (GFMC) code to leverage Mira's unique capabilities for their simulations. Both the direct calculation of neutrino scattering to the low-lying excited states of carbon-12 and the evaluation of the sum rules and response would not have been possible on Mira's predecessor, Intrepid, due to the limited amount of RAM (2 GB per node). With 16 GB of RAM per node, Mira has made it feasible to tackle such memory-intensive calculations.

The team was able to perform the most detailed simulations of the structure of the carbon nucleus to date, with their calculations of carbon-12's charge form factor and sum rules of the electromagnetic response function. These were the first simulations to consider interactions of the electromagnetic and weak currents with pairs of nucleons; previous calculations had only considered interactions with individual nucleons. The researchers determined that these pair interactions are very important to the nucleus's response.

The findings, which were published in Physical Review Letters in August 2013, will be used to evaluate the results of a recent electron scattering experiment at Jefferson Lab. The team also performed neutrino-nucleus calculations that will help enable more reliable neutrino detector calibrations and improved supernova explosion simulations. In 2014, the researchers will use an INCITE allocation to compute Euclidean response functions, which will allow for a more direct comparison with experimental data.




This graph shows longitudinal form factor: Two body terms in the density operator bring theoretical prediction closer to experimental data in the high-momentum transfer tail. The results are in good agreement with experimental data.

*Image Credit: Alessandro Lovato and Steven Pieper, Argonne National Laboratory*

**IMPACT »** These calculations are needed for the analysis of ongoing experiments, such as the electron scattering experiment at Jefferson Lab and current neutrino experiments like MiniBooNE at Fermilab. Ultimately, the simulations will lead to a better understanding of the propagation of charge and current in the nucleus and vastly improve the simple experimental models currently used for neutrino scattering by nuclei.

**PI:** William Tang | tang@pppl.gov

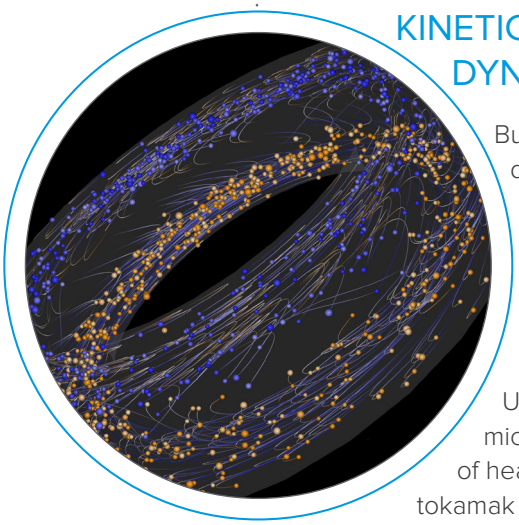
**INSTITUTION:** Princeton Plasma Physics Laboratory

**ALLOCATION PROGRAM:** INCITE/ESP

**ALLOCATION HOURS:** 40 Million/50 Million Core-Hours

**RESEARCH DOMAIN:** Physics

# KINETIC SIMULATIONS OF FUSION ENERGY DYNAMICS AT THE EXTREME SCALE



Particle visualization of a global gyrokinetic particle-in-cell simulation of microturbulence in a tokamak fusion device. This figure illustrates the dynamics of the millions of particles moving primarily in the direction parallel to the magnetic field during the simulations.

*Image Credit: Chad Jones and Kwan-Liu Ma, University of California, Davis; Stephane Ethier, Princeton Plasma Physics Laboratory*

Building the scientific foundations needed to develop fusion power demands high-physics-fidelity predictive simulation capability for magnetically confined fusion energy (MFE) plasmas. To do so in a timely way requires the development of modern software and the power of leadership-class supercomputers to simulate the complex dynamics governing MFE systems, including ITER, a multi-billion dollar international burning plasma experiment.

Unavoidable spatial variations in such systems produce microturbulence, which can significantly increase the transport rate of heat, particles, and momentum across the confining magnetic field in tokamak devices. Since the balance between these energy losses and the self-heating rates of the fusion reactions will ultimately determine the size and cost of an actual fusion reactor, understanding and possibly controlling the underlying physical processes is key to achieving the efficiency needed to help ensure the practicality of future fusion reactors.

For this INCITE project, researchers used Mira to gain new physics insights on MFE confinement scaling. The work also aimed to address the key question of how turbulent transport and associated confinement characteristics scale from present generation devices to the much larger ITER-scale plasmas.

Through decades of increasingly large tokamaks, measurements have shown that confinement losses caused by ion temperature gradient-driven instabilities become worse with increased device size. However, theory predicts that at a sufficiently large size, this trend changes and confinement becomes independent of system size. Simulations to demonstrate this so-called 'Bohm to Gyro-Bohm' transition demand high resolution to be realistic and reliable. Results from this project have revealed that the magnitude of turbulent losses is up to 50% lower than indicated by earlier simulations carried out at much lower resolution and significantly shorter duration.

**IMPACT »** Extreme-scale simulations of unprecedented spatial resolution and temporal duration have provided new scientific insights on magnetic plasma confinement. The results are accelerating progress in worldwide efforts to harness the power of nuclear fusion as an alternative to fossil fuels.

**PI:** Paul Mackenzie | mackenzie@fnal.gov

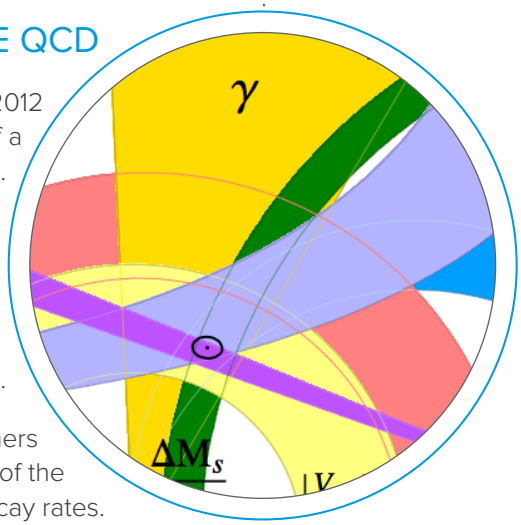
**INSTITUTION:** Fermilab

**ALLOCATION PROGRAM:** INCITE/ESP

**ALLOCATION HOURS:** 430 Million/150 Million Core-Hours

**RESEARCH DOMAIN:** Physics

## LATTICE QCD




Finding the Higgs boson at CERN's Large Hadron Collider in 2012 was a monumental discovery that confirmed the existence of a missing particle critical to the Standard Model of particle physics. But the Standard Model is still not perfect, and scientists across the world continue to search for answers to unexplained physical phenomena, such as the existence of dark matter, matter-antimatter asymmetry, and the significant discrepancy between gravity and the other fundamental forces of nature, known as the hierarchy problem.

Using a non-perturbative approach called Lattice QCD, researchers are tapping ALCF supercomputers to calculate predictions of the Standard Model for quantities such as particle masses and decay rates. The predictions can then be compared with experimental data to search for any inconsistencies that may provide evidence of physics beyond the Standard Model. With access to Mira's substantial computational power, researchers were able to give quark-antiquark pairs their proper, very light masses for the first time, removing one of the largest remaining uncertainties involved in QCD calculations.

One of the subprojects (MILC) began generating a new set of gluon configurations in 2010 to greatly reduce the errors in the simulations due to the discretization of space and time on a lattice. In April 2013, Physical Review Letters published the first work of analysis from this project. A calculation of the ratio of the decay constants of the K and pi mesons makes possible a precise determination of the ratio of two of the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements in the Standard Model, and places a stringent constraint on the scale of new physics that would alter this result. Their result is the most precise lattice-QCD determination of this ratio of decay constants, with an error comparable to the current world average.

The current summary of Lattice QCD averages.

*Image Credit: Ruth S. Van de Water, Brookhaven National Laboratory; E. Lunghi, Indiana University; Jack Laiho, Washington University in St. Louis/ University of Glasgow (Phys. Rev. D81:034503, 2010)*

**IMPACT »** This research is providing key theoretical inputs for searches of new physics beyond the Standard Model of particle physics. The project's goals are also essential for meeting milestones set out by DOE's Office of Science, providing crucial high-precision lattice QCD calculations needed for new or in-progress experiments and for analyzing results from completed experiments.

**PI:** Katrin Heitmann | heitmann@anl.gov

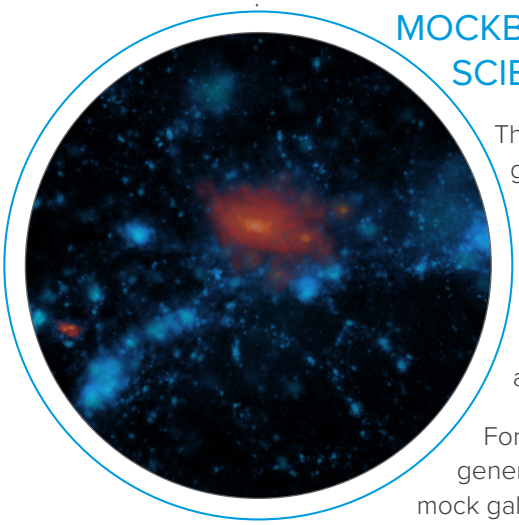
**INSTITUTION:** Argonne National Laboratory

**ALLOCATION PROGRAM:** ALCC

**ALLOCATION HOURS:** 47 Million Core-Hours

**RESEARCH DOMAIN:** Physics

## MOCKBOSS: CALIBRATING BOSS DARK ENERGY SCIENCE WITH HACC



Visualization of the dark matter distribution from one of the MockBOSS simulations. The simulation was carried out on 32,768 MPI ranks on Mira covering a cosmological volume of 5943 Mpc. The visualization shows a zoom-in to the output from only one rank, highlighting two massive dark matter clusters in red.

*Image Credit: Katrin Heitmann, Joseph Insley, Silvio Rizzi, and the HACC team, Argonne National Laboratory*

The cause of the universe's accelerated expansion is one of the great mysteries in physics today. Researchers are studying the phenomenon by mapping the large-scale structure of the universe and its growth with cosmological surveys, such as the Baryon Oscillation Spectroscopic Survey (BOSS). To analyze and interpret survey results, large-scale simulations of the universe are needed to validate the observations and serve as a defense mechanism against systematic uncertainties.

For this ALCC project, Argonne researchers are using Mira to generate a set of very large volume simulations aimed at creating mock galaxy catalogs for BOSS. The simulations are being run with HACC (Hardware/Hybrid Accelerated Cosmology Code). A major task for the analysis of the BOSS data is to develop a computationally feasible method to generate covariance matrices and explore how the covariance matrices depend on the choice of the underlying cosmological input model. A brute-force approach would require thousands of large, high-resolution simulations, which is currently not possible with available computing resources.

To develop a more manageable approach, the researchers have carried out a suite of test simulations that use a smaller number of time steps, reducing the computational time per simulations by a factor of five. These tests have shown very promising results and simulations covering the full survey are now underway. The team is exploring six different cosmological models and for each of them they are generating six simulations: one simulation at full-time resolution and five simulations with fewer time steps. These simulations are populated with galaxies to generate realistic galaxy catalogs that can be directly compared (in a statistical sense) with the observations. The fully time-resolved simulations are complete and the analysis of the results is underway.

**IMPACT »** The outcome of this research will enhance interpretation of BOSS survey data and further our theoretical understanding of the universe's accelerated expansion. The results will also deliver important insights for future surveys such as the Large Synoptic Survey Telescope. The massive volume of the simulations will enable researchers to look for rare events, such as determining the probability that a survey finds a massive cluster of galaxies in the early stage of the evolution of the universe.

# PUBLICATIONS & PROJECTS

# 2013 ALCF **PUBLICATIONS**

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

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


Wu, Xingfu, and Valerie Taylor. "Performance Modeling of Hybrid MPI/OpenMP Scientific Applications on Large-Scale Multicore Supercomputers." *Journal of Computer and System Sciences,* December 2013, vol. 79, no. 8, 1256–68.

Jiang, Wei,* James C. Phillips, Lei Huang, Mikolai Fajer, Yilin Meng, James C. Gumbart, Yun Luo, Klaus Schulten, and Benoît Roux. "Generalized Scalable Multiple Copy Algorithms for Molecular Dynamics Simulations in NAMD." *Computer Physics Communications,* December 2013, vol. 185, no. 3, 908–16.

Zhang, G.P.,* and T.F. George. "Laser-Induced Coherent Population Trapping in $C_{60}$." *Physical Review A*, December 2013, vol. 88, no. 6, 063808.

Webb, M.A., and T.F. Miller. "Position-Specific and Clumped Stable Isotope Studies: Comparison of the Urey and Path-Integral Approaches for Carbon Dioxide, Nitrous Oxide, Methane, and Propane." *Journal of Physical Chemistry A,* December 2013, vol. 118, no. 2, 467–74.

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# 2013 ALCF **PROJECTS**

## 2013 INCITE PROJECTS

### Biological Sciences

**Computational Studies of Nucleosome Stability**
George Schatz, Northwestern University
Allocation: 20 Million Core-Hours

**Multiscale Blood Flow Simulations**
George Karniadakis, Brown University
Allocation: 71 Million Core-Hours
ALCF: 20 Million; OLCF: 51 Million

**Studies of Large Conformational Changes in Biomolecular Machines**
Benoît Roux, The University of Chicago
Allocation: 55 Million Core-Hours

### Chemistry

**From LES to DNS of Explosions in Semi-Confined Domains**
Thierry Poinsot, CERFACS
Allocation: 20 Million Core-Hours

**Simulations of Deflagration-to-Detonation Transition in Reactive Gases**
Alexei Khokhlov, The University of Chicago
Allocation: 130 Million Core-Hours

**Towards Breakthroughs in Protein Structure Calculation and Design**
David Baker, University of Washington
Allocation: 140 Million Core-Hours

### Computer Science

**Developing and Testing Future Applications and Operating Systems for Exascale**
Maya Gokhale, Lawrence Livermore National Laboratory
Allocation: 50 Million Core-Hours

**Performance Evaluation and Analysis Consortium (PEAC) End Station**
Leonid Oliker, Lawrence Livermore National Laboratory
Allocation: 85 Million Core-Hours
ALCF: 40 Million; OLCF: 45 Million

**Scalable System Software for Parallel Programming**
Robert Latham, Argonne National Laboratory
Allocation: 20 Million Core-Hours

### Earth Science

**Attributing Changes in the Risk of Extreme Weather and Climate**
Michael Wehner, Lawrence Berkeley National Laboratory
Allocation: 150 Million Core-Hours

**Climate-Science Computational Development Team: The Climate End Station II**
Warren Washington, University Corporation for Atmospheric Research
Allocation: 215 Million Core-Hours
ALCF: 155 Million; OLCF: 60 Million

**CyberShake 3.0: Physics-Based Probabilistic Seismic Hazard Analysis**
Thomas Jordan, University of Southern California
Allocation: 68 Million Core-Hours
ALCF: 23 Million; OLCF: 45 Million

**Evaluation of Mesoscale Atmospheric Model for Contrail Cirrus Simulations**
Roberto Paoli, CERFACS
Allocation: 25 Million Core-Hours

### Energy Technologies

**Optimization of Complex Energy System Under Uncertainty**
Mihai Anitescu, Argonne National Laboratory
Allocation: 14 Million Core-Hours

**Thermal Hydraulic Modeling: Cross-Verification, Validation and Co-Design**
Paul F. Fischer, Argonne National Laboratory
Allocation: 50 Million-Core Hours

**Thermodynamics of Binding Biomass to Cellulases for Renewable Fuel**
Michael Crowley, National Renewable Energy Laboratory
Allocation: 70 Million Core-Hours

## Engineering

**Combustion Stability in Complex Engineering Flows**
Lee Shunn, Cascade Technologies, Inc.
Allocation: 35 Million Core-Hours

**Direct Numerical Simulations of High Reynolds Number Turbulent Channel Flow**
Robert Moser, The University of Texas at Austin
Allocation: 175 Million Core-Hours

**Enabling Green Energy and Propulsion Systems via Direct Noise Computation**
Umesh Paliath, GE Global Research
Allocation: 105 Million Core-Hours

## Materials Science

**High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry**
William George, National Institute of Standards and Technology
Allocation: 20 Million Core-Hours

**Multibillion-Atom MD Studies of the Mechanical Response of Nanocrystalline Ta**
Timothy Germann, Los Alamos National Laboratory
Allocation: 20 Million Core-Hours

**Multiscale Modeling of Energy Storage Materials**
Gregory A. Voth, The University of Chicago
Allocation: 25 Million Core-Hours

**Non-Covalent Bonding in Complex Molecular Systems with Quantum Monte Carlo**
Dario Alfé, University College London
Allocation: 95 Million Core-Hours
ALCF: 40 Million; OLCF: 55 Million

**Petascale Simulations of Stress Corrosion Cracking**
Priya Vashishta, University of Southern California
Allocation: 240 Million Core-Hours

**Predictive Materials Modeling for Li-Air Battery Systems**
Larry Curtiss, Argonne National Laboratory
Allocation: 100 Million Core-Hours

**Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces**
Giulia Galli, University of California, Davis
Allocation: 100 Million Core-Hours

## Physics

**Accelerator Simulations for the Intensity Frontier of Particle Physics**
James Amundson, Fermilab
Allocation: 80 Million Core-Hours

**Computing the Dark Universe**
Salman Habib, Argonne National Laboratory
Allocation: 40 Million Core-Hours

**Kinetic Simulations of Fusion Energy Dynamics at the Extreme Scale**
William Tang, Princeton Plasma Physics Laboratory
Allocation: 40 Million Core-Hours

**Lattice QCD**
Paul Mackenzie, Fermilab
Allocation: 430 Million Core-Hours
ALCF: 290 Million; OLCF: 140 Million

**Next-Generation Petascale Simulations of Type Ia Supernovae**
Don Lamb, The University of Chicago
Allocation: 105 Million Core-Hours

**Nuclear Structure and Nuclear Reactions**
James Vary, Iowa State University
Allocation: 155 Million Core-Hours
ALCF: 81 Million; OLCF: 74 Million

**Petascale Simulations of Inhomogeneous Alfven Turbulence in the Solar Wind**
Jean C. Perez, University of New Hampshire
Allocation: 53 Million Core-Hours

**Simulation of Laser-Plasma Interaction in National Ignition Facility Experiments**
Steven Langer, Lawrence Livermore National Laboratory
Allocation: 200 Million Core-Hours

**Spectral Slope of MHD Turbulence**
Andrey Beresnyak, Los Alamos National Laboratory
Allocation: 35 Million Core-Hours

**Three-Dimensional Simulations for Core Collapse Supernovae**
Anthony Mezzacappa, Oak Ridge National Laboratory
Allocation: 65 Million Core-Hours
ALCF: 30 Million; OLCF: 35 Million

**Transformative Simulation of Shock-Generated Magnetic Fields**
Milad Fatenejad, The University of Chicago
Allocation: 40 Million Core-Hours

## 2012-2013 ALCC PROJECTS

### Computer Science

**HPC Colony: Adaptive System Software for Improved Resiliency and Performance**
Terry Jones, Oak Ridge National Laboratory
Allocation: 3 Million Core-Hours

### Energy Technologies

**Validation Work for Heterogeneous Nuclear Reactor Calculations**
Micheal Smith, Argonne National Laboratory
Allocation: 30 Million Core-Hours

### Engineering

**Petascale Thermal-Hydraulic Simulations in Support of CESAR**
Elia Merzari, Argonne National Laboratory
Allocation: 30 Million Core-Hours

**Prediction of Multiscale, Multiphysics Turbulent Flow Phenomena Using Unstructured Large Eddy Simulation**
Parviz Moin, Stanford University
Allocation: 60 Million Core-Hours

**U.S.-Russia Collaboration on Verification and Validation in Thermal Hydraulics: Nek5000 and Conv3D Simulation of "SIBERIA" Experiment**
Aleksandr Obabko, Argonne National Laboratory
Allocation: 30 Million Core-Hours

### Materials Science

**Dynamics of Conformational Transition in Thermo-Sensitive Polymers and Hydrogels**
Subramanian Sankaranarayanan, Argonne National Laboratory
Allocation: 50 Million Core-Hours

**Liquid-Solid Interfaces in Electrocatalysis from First Principles**
Jeffrey Greeley, Argonne National Laboratory
Allocation: 20 Million Core-Hours

### Physics

**Ab Initio Hyper-Nuclear Physics**
Kostas Orginos, College of William & Mary
Allocation: 20 Million Core-Hours
ALCC: Exploring the Nature of the Lightest

**Massive Particles in the Universe**
Katrin Heitmann, Argonne National Laboratory
Allocation: 4 Million Core-Hours

## 2013-2014 ALCC PROJECTS

### Biological Sciences

**Protein Binding and Interaction Analysis of Human Pathogen Protein Targets**
T. Andrew Binkowski, Argonne National Laboratory
Allocation: 22.8 Million Core-Hours

### Earth Science

**Chombo-Crunch: Advanced Simulation of Subsurface Flow and Reactive Transport Processes Associated with Carbon Sequestration**
David Trebotich, Lawrence Berkeley National Laboratory
Allocation: 80 Million Core-Hours

**Multiscale Modeling of Dynamic Arctic Landscapes in a Changing Climate**
Richard Mills, Oak Ridge National Laboratory
Allocation: 30 Million Core-Hours

### Engineering

**Does A Turbulent Duct Flow Ever Become Two-Dimensional?**
Hassan Nagib, Illinois Institute of Technology/KTH Mechanics, Sweden
Allocation: 11 Million Core-Hours

**Petascale Thermal Hydraulic Simulations in Support of CESAR**
Elia Merzari, Argonne National Laboratory
Allocation: 80 Million Core-Hours

**U.S. Russia Collaboration on Cross-Verification and Validation in Thermal Hydraulics: Nek5000, Cfoam-CABARET, and Conv3D, Simulations of MATiS and MAX Experiments**
Aleksandr Obabko, Argonne National Laboratory
Allocation: 44 Million Core-Hours

**Wall Modeling and Primary Atomization for Predictive Large-Eddy Simulation of Airframes, Jet Engines and Jet Noise**
Parviz Moin, Stanford University
Allocation: 150 Million Core-Hours

### Materials Science

**Atomistic Simulations of Nanoscale Oxides and Oxide Interfaces**
Subramanian Sankaranarayanan, Argonne National Laboratory
Allocation: 120 Million Core-Hours

**Dynamics of Conformational Transition in Polymer Grafted Nanoparticles**
Subramanian Sankaranarayanan, Argonne National Laboratory
Allocation: 170 Million Core-Hours

**First Principles Investigations of Adsorbate-Metal Interactions: Quantum Monte Carlo and Ab Initio Molecular Dynamics Simulations**
Jeffrey Greeley, Purdue University
Allocation: 50 Million Core-Hours

**First-Principle Investigation of Oxygen Defects in Metal/Oxide/Metal Heterostructures: Structure, Energetics, and Transport in the Quantum Regime**
Olle Heinonen, Argonne National Laboratory
Allocation: 50 Million Core-Hours

**Large-Scale Computation for Discovery and Design of Excited State Phenomena in Next-Generation Energy Conversion Materials**
Jeffrey B. Neaton, Lawrence Berkeley National Laboratory
Allocation: 23 Million Core-Hours

### Physics

**Ab Initio Quantum Liquid Water and Aqueous Ionic Solutions**
Robert A. DiStasio Jr., Princeton University
Allocation: 250 Million Core-Hours

**Large Eddy Simulation of SFR Assembly Inlets**
Paul Fischer, Argonne National Laboratory; James Tallman, General Electric
Allocation: 60 Million Core-Hours

**MockBOSS: Calibrating Boss Dark Energy Science with HACC**
Katrin Heitmann, Argonne National Laboratory
Allocation: 47 Million Core-Hours

**Petascale Simulation of Laser Plasma Interactions Relevant to Inertial Fusion Energy**
F.S Tsung, University of California, Los Angeles
Allocation: 40 Million Core-Hours

**Predictive Full-Scale Simulations of Fast Ignition of Fusion Targets**
Frederico Fiuza, Lawrence Livermore National Laboratory
Allocation: 19.5 Million Core-Hours

**Understanding Helium Plasma Mediated Tungsten Surface Response that Controls Plasma Facing Component Performance and Lifetime**
Brian Wirth, Oak Ridge National Laboratory
Allocation: 7.5 Million Core-Hours

## 2013 ESP PROJECTS

### Biological Science

**Multiscale Molecular Simulations at the Petascale**
Gregory Voth, The University of Chicago
Allocation: 150 Million Core-Hours

**NAMD – The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field**
Benoît Roux, Argonne National Laboratory/The University of Chicago
Allocation: 80 Million Core-Hours

### Chemistry

**Accurate Numerical Simulations Of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC**
Robert Harrison, Oak Ridge National Laboratory
Allocation: 150 Million Core-Hours

**High-Accuracy Predictions of the Bulk Properties of Water**
Mark Gordon, Iowa State University
Allocation: 150 Million Core-Hours

**High-Speed Combustion and Detonation (HSCD)**
Alexei Khokhlov, The University of Chicago
Allocation: 150 Million Core-Hours

### Earth Science

**Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model**
Venkatramani Balaji, Geophysical Fluid Dynamics Laboratory
Allocation: 150 Million Core-Hours

**Using Multiscale Dynamic Rupture Models to Improve Ground Motion Estimates**
Thomas Jordan, University of Southern California
Allocation: 150 Million Core-Hours

### Energy Technologies

**Materials Design and Discovery: Catalysis and Energy Storage**
Larry Curtiss, Argonne National Laboratory
Allocation: 50 Million Core-Hours

**Petascale Direct Numerical Simulations of Turbulent Channel Flow**
Robert Moser, The University of Texas at Austin
Allocation: 60 Million Core-Hours

### Engineering

**Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow**
Christos Frouzakis, Swiss Fed. Inst. Tech.
Allocation: 150 Million Core-Hours

**Petascale, Adaptive CFD**
Kenneth Jansen, University of Colorado-Boulder
Allocation: 150 Million Core-Hours

### Physics

**Ab Initio Reaction Calculations for Carbon-12**
Steven C. Pieper, Argonne National Laboratory
Allocation: 110 Million Core-Hours

**Cosmic Structure Probes of the Dark Universe**
Salman Habib, Los Alamos National Laboratory
Allocation: 150 Million Core-Hours

**Global Simulation of Plasma Microturbulence at the Petascale and Beyond**
William Tang, Princeton Plasma Physics Laboratory
Allocation: 50 Million Core-Hours

**LatticeQCD - Early Science**
Paul Mackenzie, Fermilab
Allocation: 150 Million Core-Hours

**Petascale Simulations of Turbulent Nuclear Combustion**
Don Lamb, The University of Chicago
Allocation: 150 Million Core-Hours

## 2013 DD PROJECTS

### Biological Sciences

**Coarse-Grained Simulations of Sec-Facilitated Protein Translocation and Membrane Integration**
Thomas F. Miller, III, California Institute of Technology
Allocation: 6 Million Core-Hours

**Macromolecular Folding and Aggregation**
Juan de Pablo, The University of Chicago
Allocation: 2 Million Core-Hours

**Molecular Dynamics Simulations for Exploring Androgen Receptor Antagonism, Drug-Resistant Mutations, and Antagonist Design**
Yang Shen, Toyota Technological Institute at Chicago
Allocation: 3 Million Core-Hours

**Nanoscale Biomolecular Simulation for Understanding of Peptide Recognition by Epigenetic Protein**
Nadeem Vellore, The University of Utah
Allocation: 300,000 Core-Hours

**Simulation of Cell Coupling in Arterial Bifurcation**
Timothy David, University of Canterbury
Allocation: 1.1 Million Core-Hours

**Simulation of Large-Scale Biomolecular Systems**
Rommie E. Amaro, University of California-San Diego
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**Towards a Model of the Replisome**
Aleksii Aksimentiev, University of Illinois at Urbana-Champaign
Allocation: 4.2 Million Core-Hours

### Chemistry

**Investigation of Catalytic Properties of Nanocluster**
Leonardo Spanu, Shell International E&P, Inc.
Allocation: 2 Million Core-Hours

**Minimum Energy Path with Quantum Monte Carlo**
Leonardo Guidoni, University of L'Aquila
Allocation: 1 Million Core-Hours

**Probing the Free Energy Surface of Spin Separation in Singlet Fission**
Hanning Chen, The George Washington University
Allocation: 6 Million Core-Hours

**Quantum Monte Carlo Simulations of Biochemical and Catalysis-Related Systems**
William Parker, Argonne National Laboratory
Allocation: 10 Million Core-Hours

**Scaling and Baseline Study of Coupled Simulations using A Very Big Program (AVBP) on O(B) Finite Volumes on the Blue Gene/Q**
Gabriel Staffelbach, Argonne National Laboratory/ CERFACS
Allocation: 5 Million Core-Hours

### Computer Science

**Charm++ and its Applications**
Laxmikant V. Kale, University of Illinois at Urbana-Champaign
Allocation: 2.5 Million Core-Hours

**Distributed File Systems for Exascale Computing**
Ioan Raicu, Illinois Institute of Technology
Allocation: 500,000 Core-Hours

**Efficient Parallel Volume Rendering of Large-Scale Adaptive Mesh Refinement Data**
Michael E. Papka, Argonne National Laboratory
Allocation: 125,000 Core-Hours

**Open Source Compiling for Supercomputers**
Hal Finkel, Argonne National Laboratory
Allocation: 50,000 Core-Hours

## Earth Science

**Climate Sensitivity Experiments Using a Multiscale Modeling Framework with a Higher-Order Turbulence Closure in its CRM**
Anning Cheng, Science Systems and Applications, Inc./National Aeronautics and Space Administration
Allocation: 3 Million Core-Hours

**Dynamic Downscaling of Climate Models**
V. Rao Kotamarthi, Argonne National Laboratory
Allocation: 37 Million Core-Hours

**Sensitivity and Uncertainty of Precipitation of the GFDL High Resolution Model**
Laura Zamboni, Argonne National Laboratory
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## Engineering

**Aspect Ratio Effects in Turbulent Duct Flows Studied Through Direct Numerical Simulation**
Hassan Nagib, Illinois Institute of Technology/Argonne National Laboratory/KTH Royal Institute of Technology
Allocation: 1.5 Million Core-Hours

**Atomistic Simulation of Laser Processing of Metal Multilayers**
Leonid V. Zhigilei, University of Virginia
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**DNS Study of a Spatially Developing Compressible Mixing Layer with Non-Unity Density and Temperature Ratios**
Francesco Grasso, Conservatoire National des Arts et Metiers
Allocation: 2.5 Million Core-Hours

**DNS of Wall-Bounded Turbulence**
Gary N. Coleman, National Aeronautics and Space Administration
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**High-Fidelity, High-Energy-Density Hydrodynamics Simulations of Shocks Interacting with Material Discontinuities**
Eric Johnsen, University of Michigan
Allocation: 250,000 Core-Hours

**Highly Resolved LES of a GE 3-Cup Combustor System**
Anne L. Dord, General Electric Company
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**LES of Turbulent Jet Noise**
Marlene Sanjose, Universite de Sherbrooke
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**Predictive Modeling for Complex Phenomena in Electromagnetics and Fluid Systems**
Misun Min, Argonne National Laboratory
Allocation: 2 Million Core-Hours

**Porting Uintah to the Blue Gene/Q Architecture**
Martin Berzins and John Schmidt, The University of Utah
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**Quantum Lattice Algorithm for Quantum Turbulence**
George Vahala, William & Mary
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**Stochastic (w*) Convergence for Turbulent Combustion**
James Glimm, Stony Brook University
Allocation: 15.75 Million Core-Hours

## Mathematics

**Large and Accurate Numerical Solutions of Partial Differential Equations**
Benson Muite, King Abdullah University of Science and Technology
Allocation: 3 Million Core-Hours

## Materials Science

**Chemo-Mechanical Properties of Complex Oxide Interfaces**
Alessandro De Vita and James Kermode, King's College London/Argonne National Laboratory
Allocation: 2 Million Core-Hours

**LAMMPS Performance Optimization**
Paul Coffman, IBM
Allocation: 2 Million Core-Hours

**Liquid Crystal Based Functional Materials**
Juan de Pablo, The University of Chicago, Argonne National Laboratory
Allocation: 4 Million Core-Hours

**Mesoscale Modeling of Self-Assembly of Polymer Grafted Nanoparticles**
Derrick Mancini, Argonne National Laboratory
Allocation: 2 Million Core-Hours

**Nanostructure-Enhanced Detonation in Energetic Materials**
Tzu-Ray Shan, Sandia National Laboratories
Allocation: 600,000 Core-Hours

**Phonon Parallelization in Quantum ESPRESSO**
William Parker, Argonne National Laboratory
Allocation: 500,000 Core-Hours

**Radiation Tolerance and Thermo-Mechanical Properties of Amorphous SiCO Glasses and SiCO/Fe Composites**
Kan-Ju Lin, Massachusetts Institute of Technology
Allocation: 1.25 Million Core-Hours

**Toward Crystal Engineering From First Principle**
James R. Chelikowsky, University of Texas at Austin
Allocation: 1 Million Core-Hours

## Physics

**Petascale Simulation of Magnetorotational Core-Collapse Supernovae**
Sean M. Couch, The University of Chicago/Fermilab
Allocation: 30 Million Core-Hours

**Computational Studies of the Topological Properties of Micellar Solutions**
Subas Dhakal, Syracuse University
Allocation: 3 Million Core-Hours

**Diffraction-Limited Light Source for APS Upgrade**
Michael Borland, Argonne National Laboratory
Allocation: 10 Million Core-Hours

**DNS Simulations of Turbulent Convection**
Janet Scheel, Occidental College
Allocation: 1 Million Core-Hours

**First Principles Quantum Monte Carlo for Superconducting Materials**
Lucas K. Wagner, University of Illinois at Urbana-Champaign
Allocation: 500,000 Core-Hours

**Global Simulations of Accretion Discs**
Fausto Cattaneo, The University of Chicago
Allocation: 7 Million Core-Hours

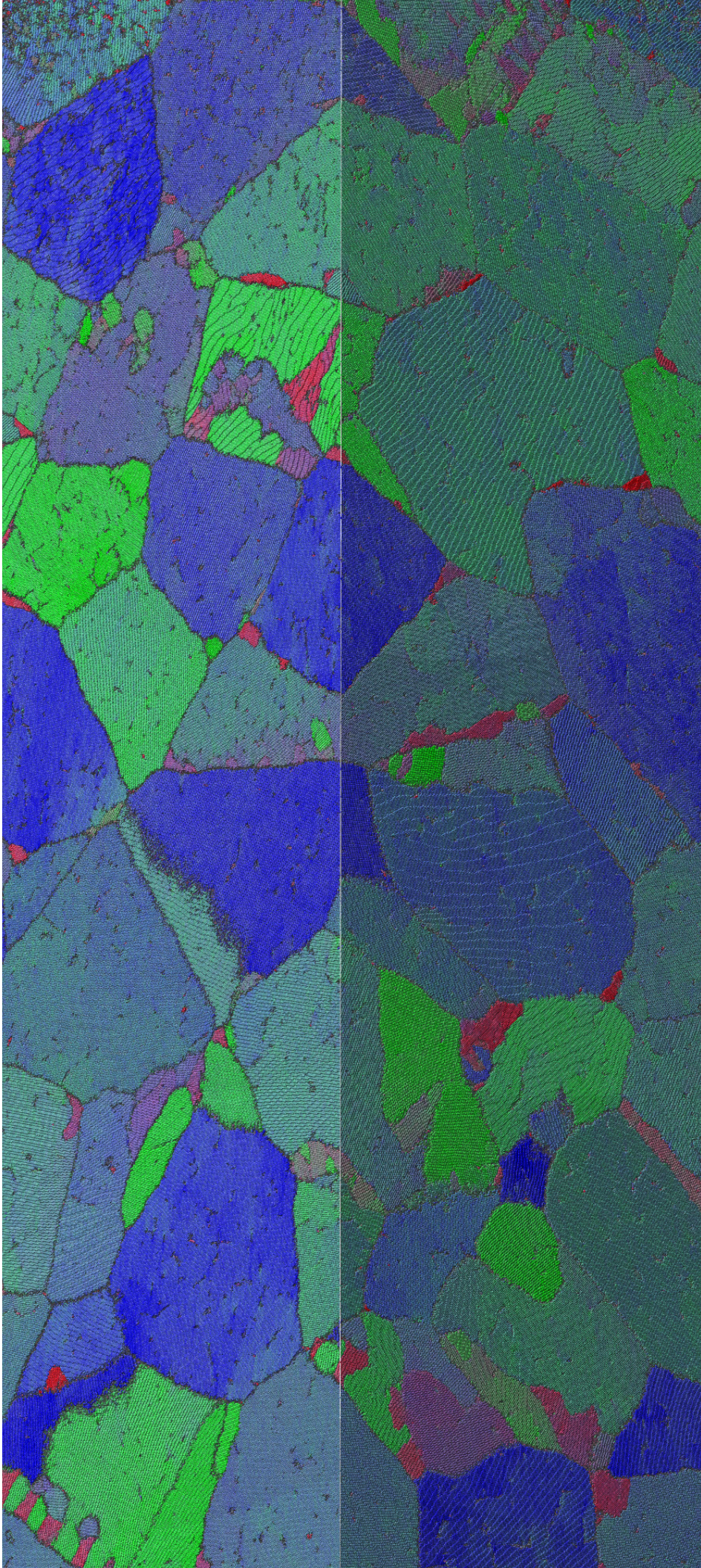
**Grid-Enabling High-Performance Computing for ATLAS**
Thomas J. LeCompte, Argonne National Laboratory
Allocation: 5 Million Core-Hours

**High-Fidelity Simulation of Small Modular Reactors with Monte Carlo**
Benoit Forget, Massachusetts Institute of Technology
Allocation: 10 Million Core-Hours

**Neutronics Simulation of FFTF and EBR-II**
Micheal A Smith, Argonne National Laboratory
Allocation: 5 Million Core-Hours

**Nuclear Structure and Nuclear Reactions**
James Vary, Iowa State University
Allocation: 1.5 Million Core-Hours

**Shearing Box Simulations of Accretion Disks**
Eric Blackman, University of Rochester
Allocation: 300,000 Core-Hours



*Plastic deformation of a shock-compressed Ta nanocrystal (323 million atoms, 50 nm grains). Atoms are colored according to their local crystallographic orientation; a shock wave is traveling from left to right, and has traveled about three-quarters of the sample length. A high density of defects form and are annealed behind the shock front, including both slip (appearing as individual points where the dislocation lines intersect the periodic boundaries on the top and front surfaces) and twinning (regions within a grain with a secondary, twin orientation color).*

*Image Credit: Tim Germann, Los Alamos National Laboratory; Ramon Ravelo, University of Texas, El Paso*

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The Leadership Computing Facility Division operates the Argonne Leadership Computing Facility—the ALCF—as part of the U.S. Department of Energy's (DOE) effort to provide leadership-class computing resources to the scientific community.

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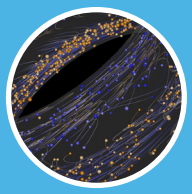
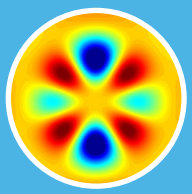


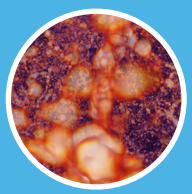
**Particle visualization of a global gyrokinetic particle-in-cell simulation of microturbulence in a tokamak fusion device.**

Image Credit: Chad Jones and Kwan-Liu Ma, University of California, Davis; Stephane Ethier, Princeton Plasma Physics Laboratory



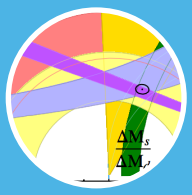
**Slice of the translationally invariant proton hexadecapole density of the ground state of $^{8}$Li, a nucleus with three protons and five neutrons. The results were calculated in the ab initio no core shell model with a realistic two-nucleon interaction.**

Image Credit: Chase Cockrell, Pieter Maris, and James P. Vary, Iowa State University



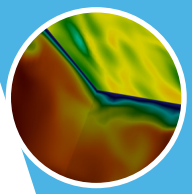
**This image shows a large simulation of the distribution of matter in the universe. The simulation was run with 1.1 trillion particles using HACC, a new simulation framework developed with the challenges of future supercomputing architectures in mind.**

Image Credit: Hal Finkel, Nicholas Frontiere, Salman Habib, Katrin Heitmann, Mark Hereld, Joseph Insley, Kalyan Kumaran, Vitali Morozov, Michael E. Papka, Tom Peterka, Adrian Pope, Venkatram Vishwanath, and Tim Williams, Argonne National Laboratory; Zarija Lukic, Lawrence Berkeley National Laboratory; David Daniel and Patricia Fasel, Los Alamos National Laboratory.



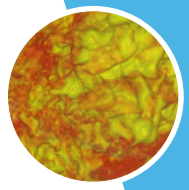
**The current summary of Lattice QCD averages.**

Image Credit: Ruth S. Van de Water, Brookhaven National Laboratory; E. Lunghi, Indiana University; Jack Laiho, Washington University in St. Louis/University of Glasgow (Phys. Rev. D81:034503, 2010)



**This 3D flow domain image depicts shear stress on the top (green) and the streamwise velocity component along the sides. The visualization is from a simulation of incompressible turbulent flow ($Re_\tau$ = 5200) between two parallel smooth planes.**

Image Credit: Myoungkyu Lee, University of Texas at Austin



**Volume renderings of the specific entropy from 3D simulations of the explosion of a 27-solar mass star.**

Image Credit: Sean Couch, The University of Chicago

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## CONTACT

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