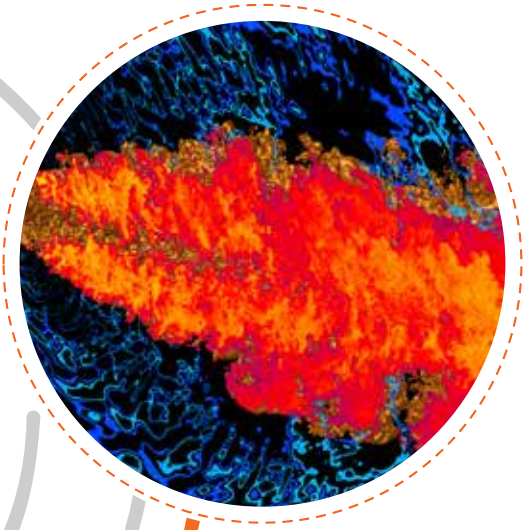
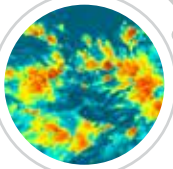
2012 annual report

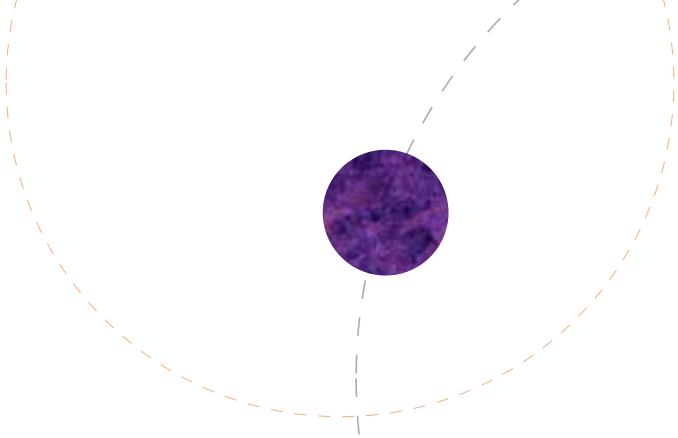
Argonne **Leadership Computing** Facility



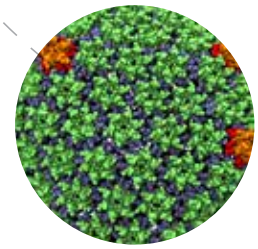


Argonne NATIONAL LABORATORY

Argonne Leadership Computing Facility



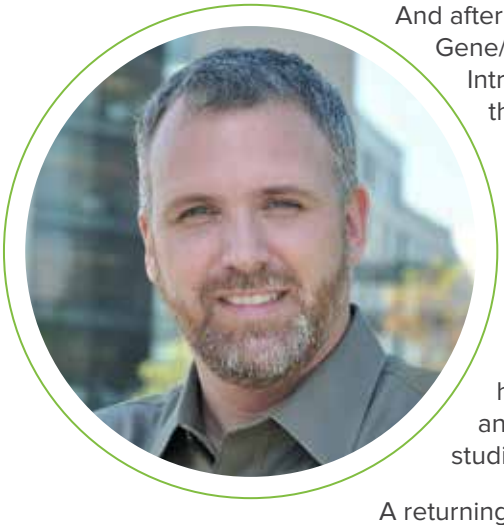
ARGONNE LEADERSHIP COMPUTING FACILITY
2012 ANNUAL REPORT



CONTENTS

MIRA
BRINGS COMPUTING AT ARGONNE INTO THE PETASCALE ERA

The Argonne Leadership Computing Facility (ALCF) had a great year, with Mira officially becoming part of Argonne's leadership class computing resources available to the nation's science and engineering community. Over the next 12 months, this petascale powerhouse will deliver billions of core hours for research.



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

And after more than four years of enabling great science, our stalwart Blue Gene/P system, Intrepid, continued to host a range of applications. Intrepid has delivered many world-changing breakthroughs, including those you will read about in the following pages, and helped advance many of the computational tools needed for the next generation of applications to take advantage of Mira's incredible capabilities.

Examples include a University of Texas at Austin research team's project aimed at designing new crystalline materials that have application ranging from drug design to hydrogen storage. The team used its Director's Discretionary allocation to develop a highly accurate and efficient method for describing the structure and energetics of molecular crystals, and applied it to several case studies.

A returning team from University of Southern California used its INCITE allocation to run larger and more detailed simulations of the atomistic mechanisms that control stress-induced corrosion within nuclear reactors—advancing the body of knowledge needed to understand the phenomenon, and ultimately, to develop new technologies to prevent it. On Mira, the team will attempt simulations that encompass several billion atoms for nanosecond timescales, and several million atoms for microseconds.

A Stanford University team used its ASCR Leadership Computing Challenge allocation to make a major discovery about crackle, the dominant (and deafening) component of jet noise. The team ran large eddy simulations to pinpoint the source of crackle in hot supersonic jet engines. Now new nozzle designs can be simulated using Mira to help meet the U.S. Navy's near-term jet noise reduction goal.

Looking towards the future, an Early Science Program team led by Argonne physicists has already run the largest, most complex simulation of the large-scale structure of the universe ever undertaken—a 1.1-trillion-particle simulation run on half a million processor cores of Mira—to create the largest "man made" universe ever.

The ALCF has the experience and expertise to accelerate a wide range of discoveries on our leadership class systems. We look forward to witnessing how the next generation of science teams will push the limits of computing power yet again.

▲ ALCF Director Michael Papka shows U.S. Congressman Bill Foster the inner workings of Mira during a tour of the facility's machine room.

ABOUT ALCF

The Argonne Leadership Computing Facility provides researchers from national laboratories, academia, and industry with access to high-performance computing capabilities dedicated to 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 for humanity by designing and providing world-leading computing facilities in partnership with the computational science community.

According to the TOP500 list, Mira ranked as the third fastest supercomputer in June and the fourth fastest in November. Mira achieved 8.1 petaflops on the LINPACK benchmark, using 786,532 processing cores on 48 racks.

On the Graph 500 list, Mira tied for first place in June and ranked second in November, achieving 10,461 GTEPS (giga traversed edges per second) with its latest score.

Blue Gene/Q systems held the top 10 spots on the Green500 in June and six of the top 10 spots in November. This biannual list ranks the top 500 supercomputers in the world by energy efficiency.

INTRODUCING MIRA

With the launch of Mira, a new 10-petaflops supercomputer, the ALCF will open the door for researchers and industry to analyze data more efficiently, design products more quickly, and address some of society's biggest problems in ways that would otherwise be impossible.

Currently ranked as the fourth fastest computer in the world, Mira, an IBM Blue Gene/Q system, is capable of 10 quadrillion calculations per second. With this computing power, Mira can do in one day what it would take an average personal computer 20 years to achieve.

As supercomputers continue to improve, so do the results. Faster and more sophisticated computers mean better simulations and more accurate predictions. Mira will help researchers to tackle more complex problems, achieve faster times to solutions, and create more robust models of everything from jet engines to the human body.

Consisting of 48 racks 786,432 processors, and 768 terabytes of memory, Mira is 20 times faster than Intrepid, its IBM Blue Gene/P predecessor at the ALCF. Mira was grown from the same DNA as Intrepid, but features many revolutionary advances.

As a machine for open science, any researcher with a question that requires large-scale computing resources can submit a proposal for time on Mira, typically in allocations of millions of core-hours, to run programs for their experiments. This adds up to billions of hours of computing time per year.

In addition to being one of the fastest computers in the world, Mira is also among the most energy efficient. The supercomputer saves considerable energy through innovative chip designs and a unique water-cooling system.

By fitting more cores onto a single chip, Mira speeds the communication between cores and saves the energy lost when transporting data across long distances. Mira's water-cooling system uses copper tubes to pipe cold water directly alongside the chips, saving power by eliminating an extra cooling step. Overall, the new system operates five times more efficiently than Intrepid, and roughly within the same footprint.

Beyond enabling scientific discoveries in a sustainable way, Mira itself is a stepping stone toward the next great goal of supercomputing: exascale speed, where computers will operate a thousand times faster than today's top machines.

ALCF CONTRIBUTES TO CO-DESIGN OF MIRA

The future scientific breakthroughs enabled by Mira may not be its only legacy. Argonne National Laboratory worked closely with IBM Research and Lawrence Livermore National Laboratory to design and develop the hardware and software that make up Mira's IBM Blue Gene/Q architecture. This successful co-design effort serves as a model for the development of new supercomputers, including future exascale systems.

From the outset of the co-design process in 2007, the intent was to design a supercomputer with low power requirements and very high scalability. This highly collaborative approach brought a wealth of expertise and perspectives to the table, resulting in many detailed discussions and analyses of the costs and benefits of various hardware and software configurations. The process involved weighing the tradeoffs of key architectural decisions such as the number of processors, the amount of memory cache, and the type of network topology.

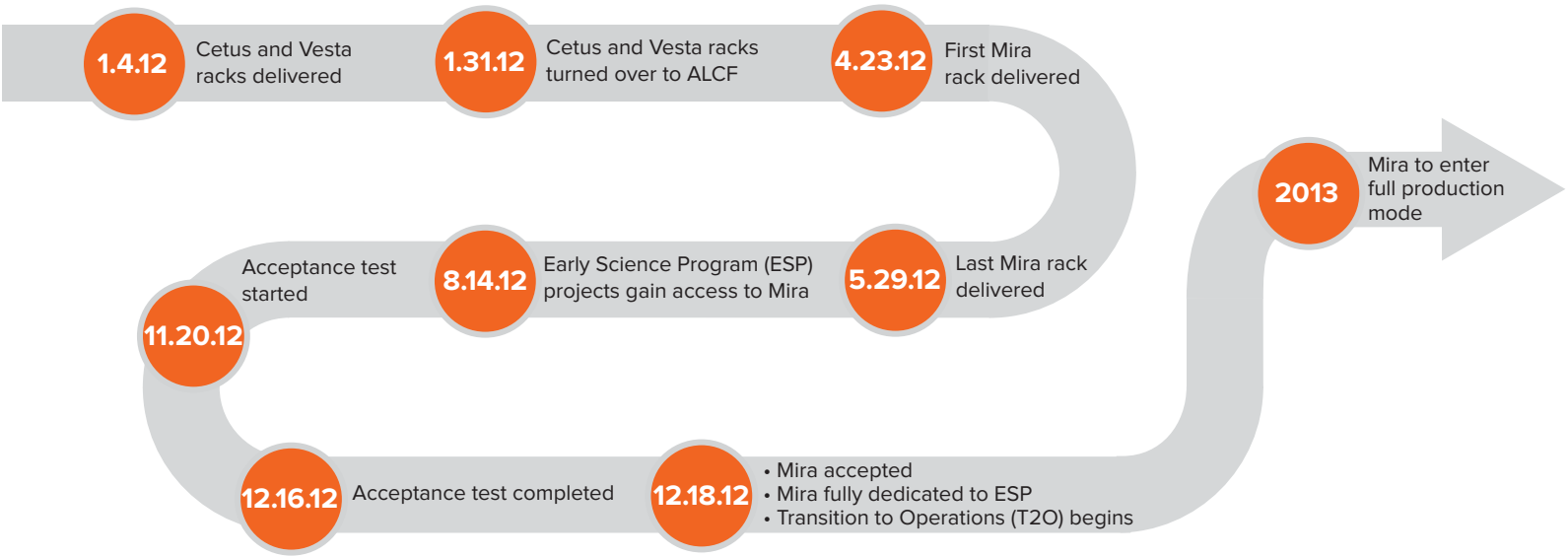
Drawing on deep expertise with many applications, the Argonne team (made up of staff from the ALCF and the Mathematics and Computer Science Division) was able to convey the needs of its future users, and assess system features relevant to applications that would ultimately run on the machine. In the end, the co-design resulted in state-of-the-art hardware that was designed to meet key application needs, and, in turn, applications were tuned to take advantage of the Blue Gene/Q's unique features. The ALCF's Early Science Program confirmed that porting applications from the Blue Gene/P supercomputer to the Blue Gene/Q system often required little or no modification, and resulted in substantial performance increases over the same number of Blue Gene/P nodes.

The unique co-design partnership was formed as part of design and prototype R&D project jointly funded by IBM, the U.S. Department of Energy's (DOE) Advanced Scientific Computing Research program within the Office of Science, and the Advanced Simulation and Computing program within DOE's National Nuclear Security Administration. IBM's two predecessor systems, the Blue Gene/P and Blue Gene/L supercomputers, were also developed through co-design efforts with IBM and DOE. IBM was recognized with a National Medal of Technology and Innovation in 2009 for the development of its Blue Gene family of supercomputers.

BLUE GENE/Q ARCHITECTURAL INNOVATIONS

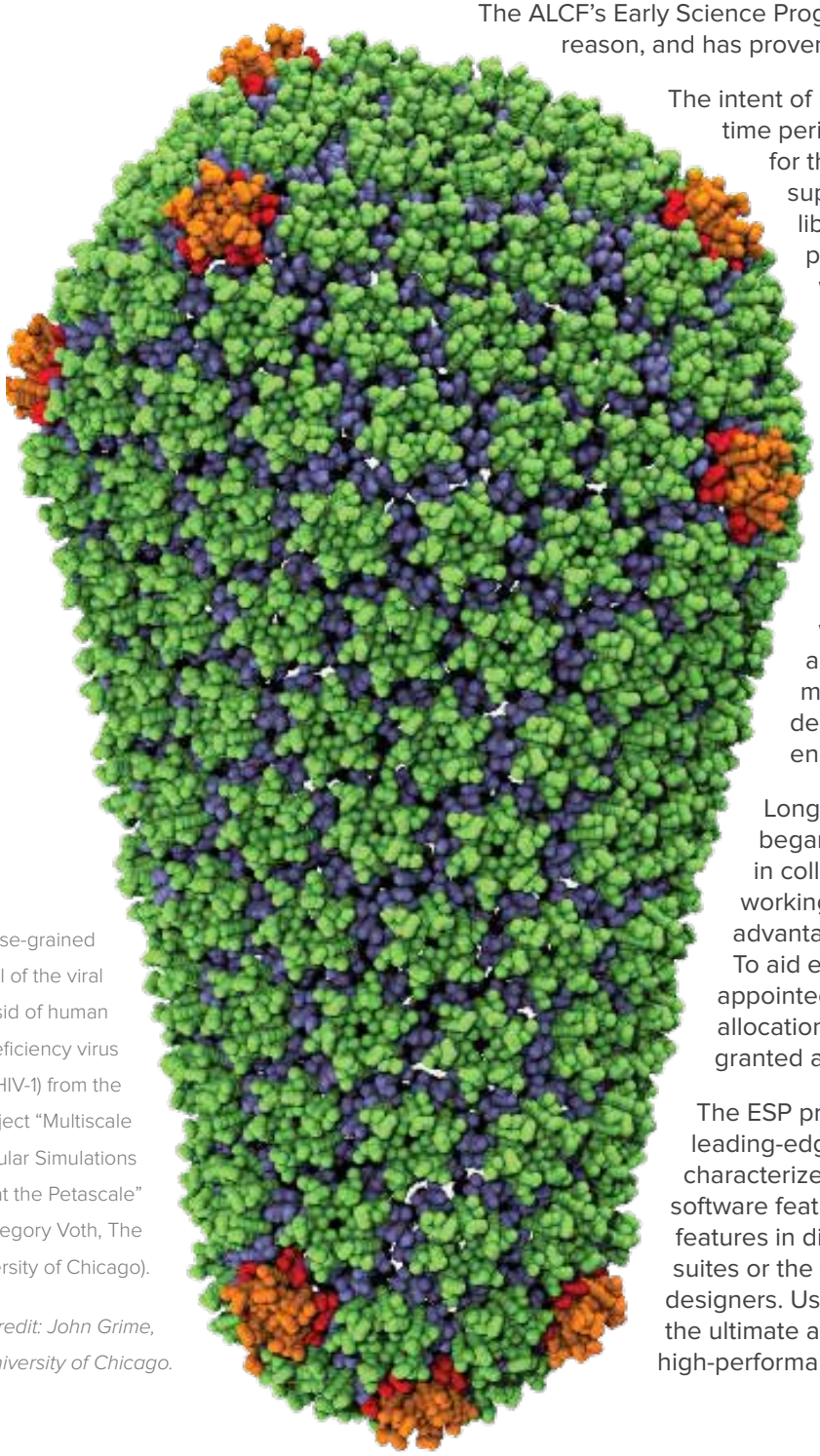
- Programmable level 1 cache data prefetching units reduce memory access latency, improve computational speed, and enable management of data and computation flow.
- An enhanced 5D integrated torus network enables reduced latency and shorter communication paths.
- High-performance quad floating-point SIMD (single-instruction, multiple-data) units enhance computational speed with improved floating-point throughput.
- The first production supercomputer with hardware support for transactional memory and speculative execution. This expands opportunities for concurrent execution and reduces compute time with thread-level, out-of-order execution.
- Hardware threads for node-level parallelism improve the scheduling of thread execution, enable level 2 cache features for smart thread queuing, and reduce synchronization costs with an on-chip wake-up unit.

MIRA 2012
FROM INSTALLATION TO OPERATIONS



SCIENCE ON DAY ONE

To hit the ground running with Mira, it was essential to be prepared to use the supercomputer for leadership-level research as soon as possible after installation. The ALCF's Early Science Program (ESP) was established for this very reason, and has proven to be a great success.



Coarse-grained model of the viral capsid of human immunodeficiency virus type 1 (HIV-1) from the ESP project "Multiscale Molecular Simulations at the Petascale" (PI: Gregory Voth, The University of Chicago).

Image Credit: John Grime, The University of Chicago.

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. When the program launched in 2010, 16 projects were selected to participate and were awarded a combined two billion core-hours on Mira. In addition to their plans to deliver new science, the 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 ESP projects formed a representative sample of the science domains present in the ALCF workload, including science to simulate advanced materials, explore the universe, model biological systems, and further the design of new, safe, and reliable sources of energy.

Long before the first pieces of Mira hardware began arriving at Argonne, ESP project teams, in collaboration with ALCF and IBM staff, started working to adapt their software to take full advantage of Mira's Blue Gene/Q architecture. To aid efforts, the ALCF appointed a postdoctoral appointee to each team, provided modest allocations on Intrepid (Mira's predecessor), and granted access to prototype systems.

The ESP projects helped to tease out bugs that leading-edge systems inevitably have and to characterize the behavior of new hardware and software features. Scientific applications use system features in different ways than standard benchmark suites or the tests provided by the computer designers. Using "real apps" has long been considered the ultimate approach for shaking out quirks in new high-performance computing systems.

ESP project participants, in collaboration with ALCF catalysts and performance engineers, did identify some early hardware and software issues. For example, ESP applications were able to dig into the software stack and pinpoint performance bottlenecks and bugs in the pre-release system software. IBM's highly responsive and dedicated hardware and software engineers quickly addressed these issues, helping to prepare Mira for acceptance and operations.

In addition to the 16 ESP science projects, a related project, "Enabling Petascale Science on BG/Q: Tools, Libraries, Programming Models, & Other System Software," was specifically dedicated to developing, porting, and installing software on Mira. This collaborative effort resulted in 15 libraries, 12 performance tools, five programming models, and two vendor debuggers being immediately available on Mira. Having these software tools ready to go at the beginning of the system's life will contribute to the success of all research projects on Mira.

EARLY RETURNS

MIRA'S IMPACT ON ESP

The ALCF's 16 ESP projects pursued real scientific problems, while simultaneously vetting the system and gathering knowledge to prepare future projects for Mira's vastly increased power and capabilities. On pages 8-9, we provide examples of how some ESP projects have leveraged the Blue Gene/Q innovations noted below to accelerate science (icons for each Mira feature are listed with relevant projects). The accomplishments represent early project results as ESP work continues into 2013.

KEY MIRA FEATURES:

Node-Level Parallelism improves performance with multi-threading. With 16 cores on a node, each of which can execute four hardware threads, the system node has a total concurrency of 64.

Level 1 Cache Data Prefetching Units reduce memory access latency, improve computational speed, and enable management of data and computation flow.

Level 2 Cache Atomics provides fast synchronization and concurrent data structures for high intranode performance of various codes.

Quad Processing Extensions (QPX) allow each core to execute four-wide SIMD floating-point instructions on double precision values, or two-wide SIMD on complex doubles.

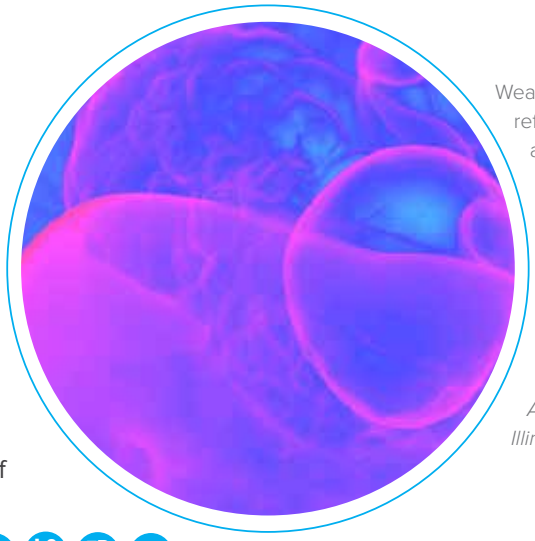
5D Torus Interconnect enables highly efficient communication by reducing the average number of hops and latency between compute nodes.

System Balance of communication, memory access, threading, and single-core processing speed enables scalable performance.

High-Speed Combustion and Detonation

Alexei Khokhlov, The University of Chicago

This project is tapping Mira to simulate the high-speed combustion and detonation of hydrogen-oxygen mixtures to enable the design of safer hydrogen fuel systems. Mira has made it possible to resolve the theory of hydrogen detonation and conduct first-principles, direct numerical simulations of the deflagration-to-detonation transition.



Weak ignition behind a reflected Mach=1.5 shock in a stoichiometric hydrogen-oxygen mixture at 0.1 atm initial pressure.

Image Credit: Charles Bacon, Argonne National Laboratory; Alexei Khokhlov, University of Chicago; Joanna Austin and Andrew Knisely, University of Illinois at Urbana-Champaign.

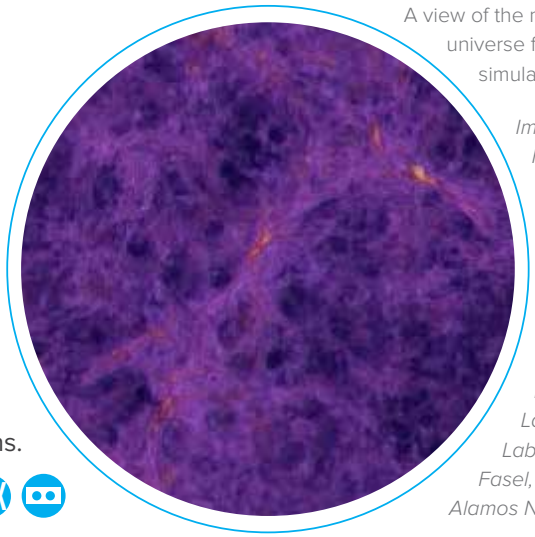
ACCOMPLISHMENTS ON MIRA

- First simulations to observe weak ignition in $2H_2$-O_2, achieving excellent agreement with experimental studies (prior to Mira, simulations did not have the resolution or scale needed for such observations).
- Improved performance by 2.5x per core (compared to Blue Gene/P), resulting in faster time-to-solution.

Cosmic Structure Probes of the Dark Universe

Salman Habib, Argonne National Laboratory

Researchers are using Mira to simulate the distribution of matter in the universe to improve our understanding of dark energy and dark matter. These simulations will shed new light on the true nature of the universe by helping us to better understand and interpret high-resolution experimental observations.



A view of the matter distribution in the universe from a 1.1 trillion-particle simulation.

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

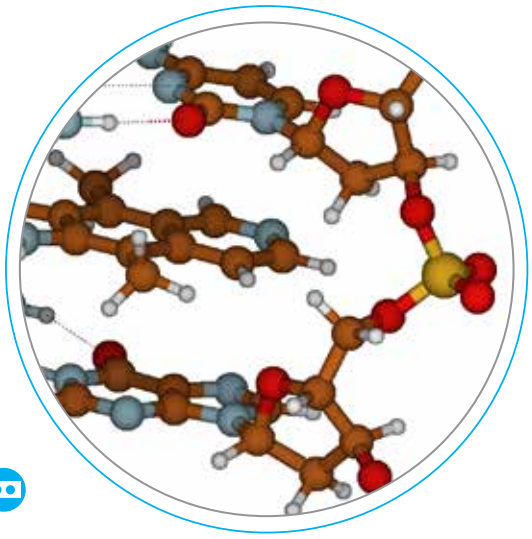
ACCOMPLISHMENTS ON MIRA

- Performed the largest, most complex simulations of the universe attempted to date.
- For the first time, these simulations delivered the required 1% error-bars to compare with state-of-the-art sky surveys.
- Improved performance of the HACC code has resulted in faster time-to-solution using 6.5x total memory of the Blue Gene/P system.

Improving Cancer Drug Design through Quantum Chemistry

Larry Curtiss and Anouar Benali, Argonne National Laboratory

This project is pairing the power of Mira with newly available electronic structure codes to conduct massively parallel quantum mechanical calculations for use in the design of materials, including improving the effectiveness of ellipticine, a promising new drug for uterine cancer treatment.



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

Image Credit: Anouar Benali, Argonne National Laboratory.

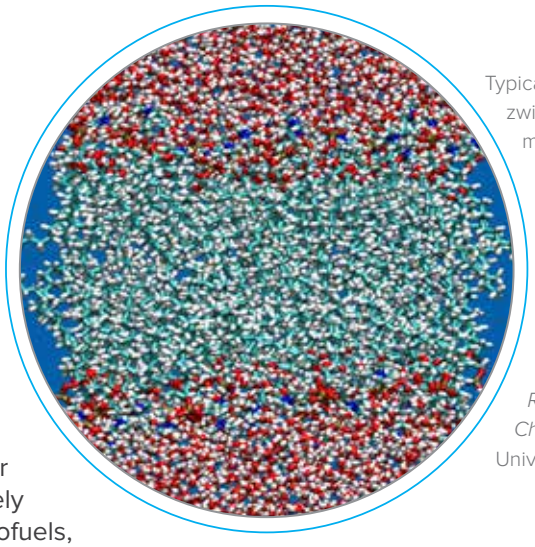
ACCOMPLISHMENTS ON MIRA

- Characterized the drug's binding energies, providing critical input for improved modeling.
- Performed accurate noble gas simulations using quantum Monte Carlo (QMC) for the first time (prior to Mira, only experimental results were available).
- Proved that many molecules thought to be too complicated or too large for quantum chemistry can be tackled by QMC methods.
- Achieved 2.68x time-to-solution speedup with the QMCPACK code (compared to Blue Gene/P), making an accurate, but expensive technique more tenable for future use.

NAMD – The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field

Benoit Roux, The University of Chicago

Researchers are applying advanced strategies based on large-scale molecular dynamics (MD) simulations to create virtual models of biomolecular systems with unprecedented accuracy. Results aim to further our understanding of the molecular mechanics of transporting materials, ultimately improving how we design drugs, produce biofuels, and conduct other important processes.

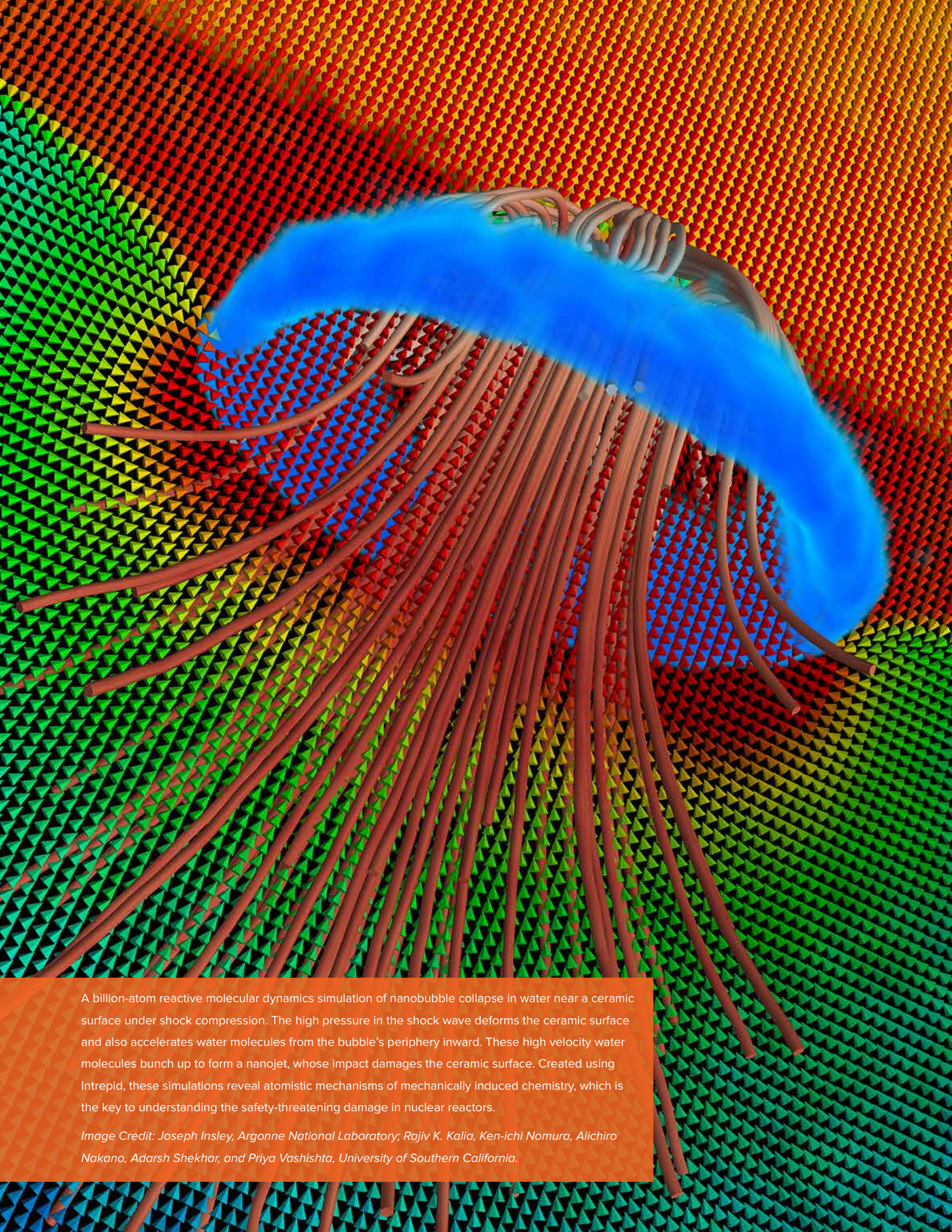


Typical configuration of a zwitterionic lipid bilayer membrane. A polarizable force field is essential for meaningful simulations of such a system.

Image Credit: Janamejaya Chowdhary, Wei Jiang, Yun Luo, and Benoit Roux, The University of Chicago; Alex MacKerell, University of Maryland.

ACCOMPLISHMENTS ON MIRA

- Completed a study of G-actin protein that was key to understanding how cells store and use energy through adenosine triphosphate.
- Protein changes proven to be in excellent agreement with experimental data.
- Achieved 20% speedup of NAMD code (compared to Blue Gene/P).



A billion-atom reactive molecular dynamics simulation of nanobubble collapse in water near a ceramic surface under shock compression. The high pressure in the shock wave deforms the ceramic surface and also accelerates water molecules from the bubble's periphery inward. These high velocity water molecules bunch up to form a nanojet, whose impact damages the ceramic surface. Created using Intrepid, these simulations reveal atomistic mechanisms of mechanically induced chemistry, which is the key to understanding the safety-threatening damage in nuclear reactors.

Image Credit: Joseph Insley, Argonne National Laboratory; Rajiv K. Kalia, Ken-ichi Nomura, Aiichiro Nakano, Adarsh Shekhar, and Priya Vashishta, University of Southern California.

RESOURCES & EXPERTISE

ALCF COMPUTING RESOURCES

MIRA SPECS

16 — 1600 MHz PowerPC A2 CORES

RACKS — 48

49,152 — NODES

CORES — 786,432

16 GB — RAM Per Node

Torus Interconnect — 5D

384 — I/O NODES

PEAK PERFORMANCE of — 10 Petaflops

ALCF Blue Gene/Q Systems

MIRA. Mira, the ALCF's Blue Gene/Q supercomputer, is equipped with 786,432 cores, 768 terabytes 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 the communication library. 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 floating point unit (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 16 1600 MHz PowerPC A2 cores, two racks, 2,048 nodes, 16 GB RAM per node, 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 16 1600 MHz PowerPC A2 cores, one rack, 1,024 nodes, 16 GB RAM per node, 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) 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 28.8 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 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 public network connectivity. Scientists can transfer datasets to and from other institutions over fast research networks such as the Energy Science Network (ESNet) and Internet2.

▲ In Mira, copper tubes pipe cold water directly alongside the chips, which saves power by eliminating an extra cooling step.

INTREPID SPECS

4 — 850 MHz PowerPC **450 CORES**

RACKS — **40**

40,960 — **NODES**

CORES — **163,840**

2 GB — **RAM** Per Node

Torus Interconnect — **3D**

640 — **I/O NODES**

PEAK PERFORMANCE of **0.5 Petaflops**

ALCF Blue Gene/P Systems

INTREPID. Intrepid, the ALCF's Blue Gene/P supercomputer, consists of 40 racks, 163,840 cores, 40,960 nodes, 80 terabytes 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 4,096 cores, 1,024 nodes, 2 GB RAM per node, 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 GB RAM per node, 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 is the Blue Gene/P 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 public 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).

◀ ALCF performance engineer Scott Parker leads a group of DOE Graduate Student Fellows on a tour of the ALCF's machine room. Here, Parker displays a tray of terabyte disk drives that make up part of Intrepid.

EXPERTISE
AT THE ALCF

Skilled experts at the ALCF enable researchers to conduct breakthrough science on the Blue Gene systems in key ways.

ALCF management: (clockwise from left): Michael Papka, ALCF Director; Bill Allcock, Director of Operations; Richard Coffey, Director of User Experience; Paul Messina, Director of Science; and Susan Coghlan, ALCF Deputy Director.

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.

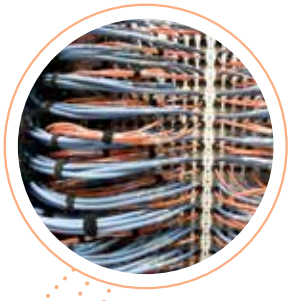
Performance Engineers help users achieve optimal performance on ALCF resources by working with them to port, tune, and parallelize scientific applications and other software. This includes assessing and improving the algorithms used by applications and the techniques used to implement those algorithms.

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.

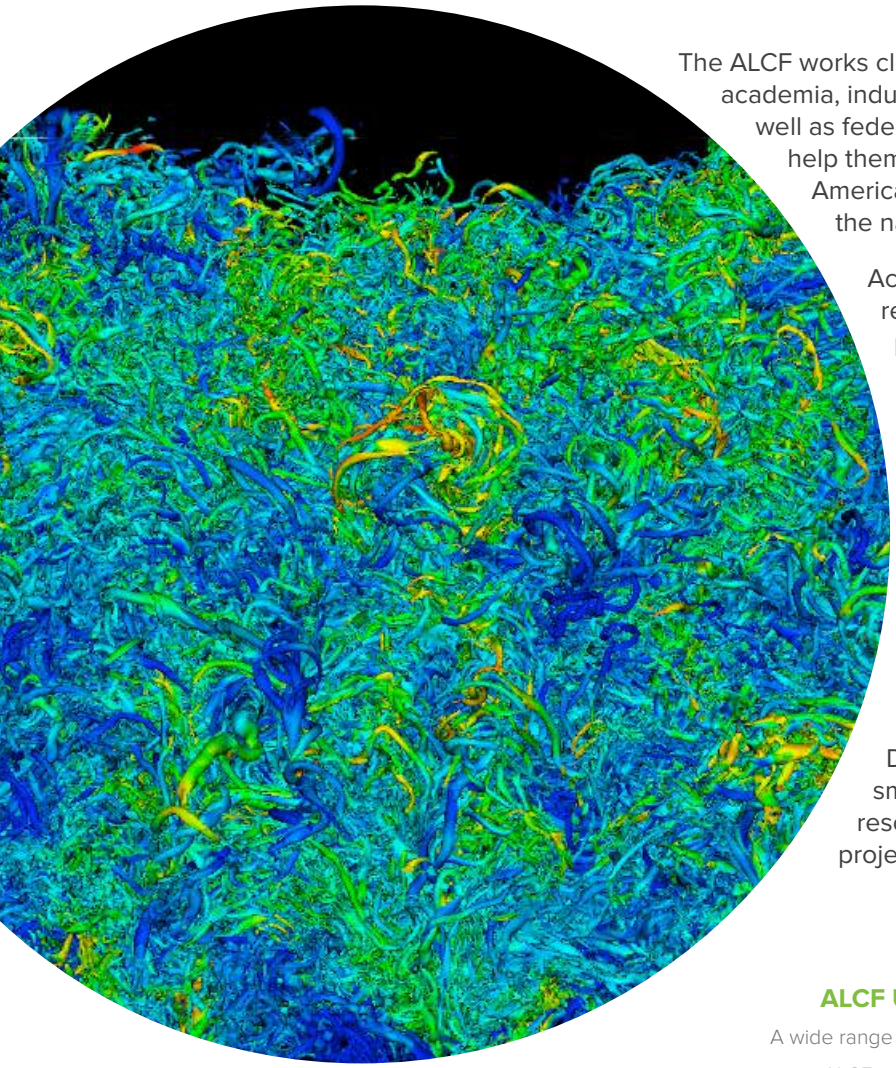
Operations ensures that system hardware and software work reliably and optimally; system tools are matched to the unique system architectures and scale of ALCF resources; the entire system software stack works smoothly together; and I/O performance issues, bug fixes, and requests for system software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

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

▲ Expert staff helps researchers maximize ALCF resources and achieve the best applications performance, accelerating key scientific discoveries and engineering breakthroughs for humanity.



ALLOCATION PROGRAMS
INCITE, DIRECTOR'S DISCRETIONARY, ALCC AND EARLY SCIENCE



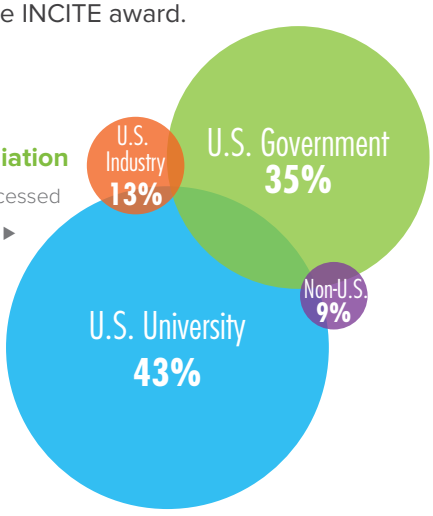
▲ A snapshot of a Richtmyer-Meshkov instability simulation from the INCITE project "Turbluent Multi-Material Mixing in the Richtmyer-Meshkov Instability." *Image Credit: Sanjiva K. Lele and Santhosh K. Shankar, Stanford University.*

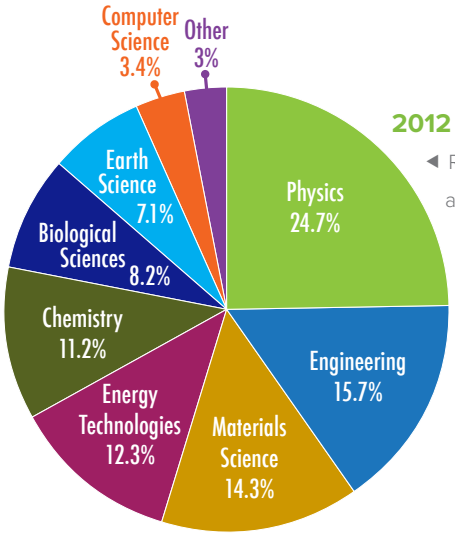
The ALCF works closely with researchers from academia, industry, and national laboratories—as well as federal, state, and municipal agencies—to help them solve complex challenges, advance America's scientific leadership, and prepare the nation for a better future.

Access to the ALCF's computing resources is available for research primarily through DOE Office of Science allocation programs. Approximately 60 percent of ALCF resources are awarded to researchers with computationally intensive, large-scale research projects through DOE's INCITE program. The DOE ASCR Leadership Computing Challenge (ALCC) program allocates 30 percent of ALCF resources. Researchers may also apply for time through the ALCF-managed Director's Discretionary program, a smaller initiative (about 10 percent of resources) designed to prepare smaller projects for a future INCITE award.

ALCF Users by Affiliation

A wide range of institutions accessed ALCF resources in 2012. ▶





2012 INCITE by Domain

◀ Researchers from a wide range of disciplines were awarded a total of 732 million core-hours on Intrepid through the INCITE program in 2012.

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

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

ASCR Leadership Computing Challenge (ALCC) Program

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.

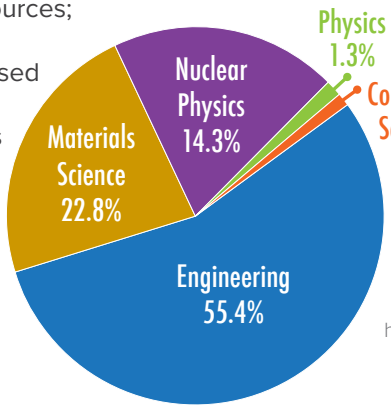
Director's Discretionary Program

The Director's Discretionary program provides "start up" awards to researchers working toward an INCITE or ALCC allocation so that they can 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 tens of thousands to the low millions of hours.

Early Science Program (ESP)

Allocations through the ESP awarded researchers with pre-production hours (between system installation and full production) on Mira. This early science period provided projects a significant head start for adapting to the new machine and access to substantial computational time, while allowing them to pursue real scientific problems. During this shakedown period, users assisted in identifying the root causes of any system instabilities, and work with ALCF staff to help develop solutions. Two billion core-hours were allocated through ESP.

Please visit alcf.anl.gov/programs for more information on how to get an allocation at the ALCF.



2012 ALCC by Domain

◀ Researchers pursuing DOE mission-related projects were awarded a total of 307 million core-hours on Intrepid through the ALCC program in 2012.

RUNNING INTREPID, PREPARING FOR MIRA

Paul Messina

Director of Science, ALCF

While 2012 will be remembered as the year we stood up Mira, it should also be remembered as another banner year for science at the ALCF. We delivered 1.2 billion core hours of compute time on Intrepid, our Blue Gene/P supercomputer. I'm pleased to report that about two-thirds of that time was consumed by "capability" jobs, i.e., ones that require at least 20 percent of the machine cores to run. We set targets for capability jobs to ensure that our supercomputers are being used by projects that require large-scale leadership computing systems. In 2012, we far exceeded our 40 percent capability usage target for INCITE projects with an impressive 63 percent of INCITE hours being run at capability.

The resulting science was also impressive, with ALCF research leading to more than 150 publications, many of which appeared in high-impact scientific journals. From improving the safety of hydrogen fuel to enabling the power grid to take better advantage of renewable energy sources, Intrepid supported 31 INCITE and 9 ALCC projects pursuing a wide variety of scientific and engineering breakthroughs in 2012. And this doesn't count the 16 projects that began to tap Mira as part of our Early Science Program (ESP), which has proven to be a runaway success that could potentially serve as a model for other supercomputing facilities planning to launch new machines.

Running Intrepid at full bore while simultaneously preparing to launch Mira is no small feat. Our high-performance computing systems may be the engines that drive computational research at our facilities, but it's our dynamic staff that empowers ALCF users to get the most of these machines. Our catalysts and performance engineers pulled double duty this year, working closely with researchers on Intrepid while also pushing ESP projects forward on Mira. Our User Services and Operations staff also played critical – though less visible – roles in enabling the computational research that is carried out on ALCF system.

In the following pages, we highlight 24 projects that used our facility in 2012. As we've done in the past, we selected a sampling of projects to represent a variety of scientific disciplines and allocation types (INCITE, ALCC, Director's Discretionary, and ESP).

SCIENCE HIGHLIGHTS

PI: T. Andrew Binkowski

INSTITUTION: Argonne National Laboratory

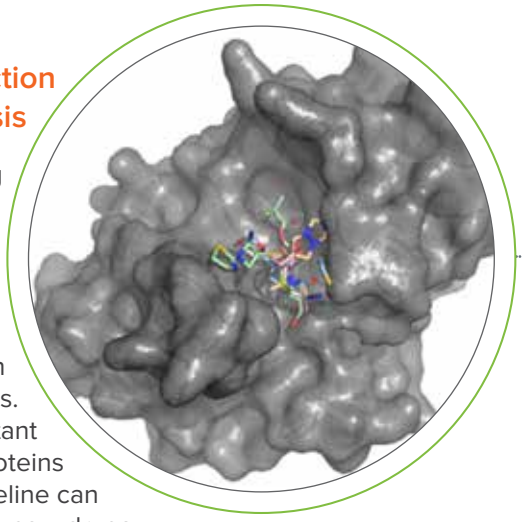
ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 10 Million Core-Hours

RESEARCH DOMAIN: Biological Sciences

Protein-Ligand Interaction Simulations and Analysis

At their most basic, disease-fighting pharmaceuticals consist of small molecules that bind to a protein pathogen and alter or disrupt the enzymes that permit it to grow. But drug design is time-consuming work, and moving a drug through the approval process can take years. Keeping pace with antibiotic-resistant strains is a challenge when proteins adapt more quickly than the pipeline can supply new drugs.



Advanced docking simulations of existing antibiotics (shown in stick form) provide insight on the antibiotic resistance of the NDM-1 enzyme (gray).

Image Credit:
T. Andrew Binkowski,
Argonne National Laboratory/
The University of Chicago.

NDM-1, a gene found in many drug-resistant bacteria, presents just such a challenge. But a University of Chicago and Argonne National Laboratory research team led by Andrew Binkowski is using the power of supercomputers to analyze NDM-1 to determine why it makes bacteria so drug-resistant. Over the course of one month, Binkowski's team studied nine compounds—a substantial speed-up over conventional experiments that would have taken months to obtain results.

Using supercomputers, scientists are gaining valuable insight into developing strategies to combat this public-health threat.

Contact: abinkowski@anl.gov

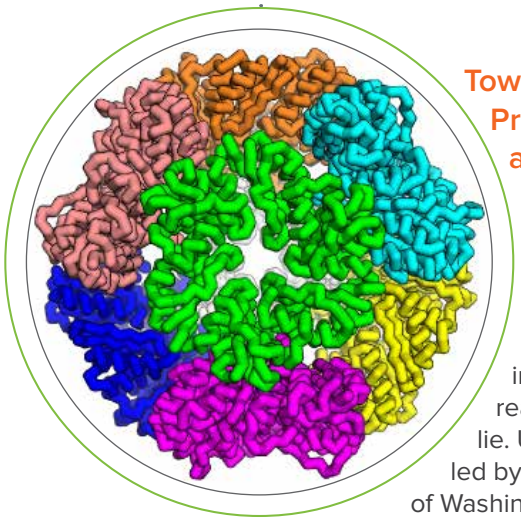
PI: David Baker

INSTITUTION: University of Washington

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 33 Million Core-Hours

RESEARCH DOMAIN: Biological Sciences



The crystal structure and design model for a self-assembling cage designed using Rosetta. Such self-assembling nanomaterials could become the basis for a next generation of vaccines and drug delivery vehicles.

Image Credit: Neil King, University of Washington.

Towards Breakthroughs in Protein Structure Calculation and Design

Computation has become an indispensable tool for conducting biomedical investigations. Protein structure prediction is key to understanding the function and interactions of biomolecules—the realm where foundational advances lie. Using ALCF resources, a team led by David Baker of the University of Washington has developed high-resolution protein structure prediction tools to build models of proteins with atomic-level accuracy and to computationally engineer both proteins and enzymes with new functions for applications ranging from basic research to therapeutics to bioremediation.

Baker's landmark structural prediction and design computer program, Rosetta, will help solve structures of biologically important proteins for which experimental X-ray phases are not available or are hard to obtain.

Using very sparse experimental data sets, the team has been able to determine the structures of many proteins of biological interest; design novel enzymes catalyzing new chemistries; design small proteins that block influenza virus infection; and design self assembling protein nanomaterials. Their research promises to advance the disciplines of biomedicine and biotechnology.

Contact: dabaker@u.washington.edu

PIs: Donald Truhlar, Osanna Tishchenko

INSTITUTION: University of Minnesota

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 15 Million Core-Hours

RESEARCH DOMAIN: Chemistry

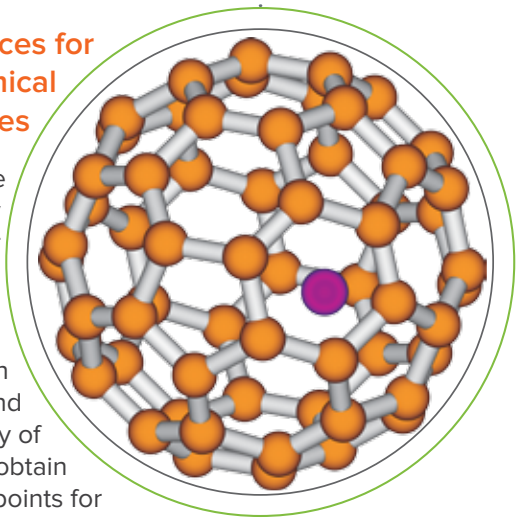
Potential Energy Surfaces for Simulating Complex Chemical Processes

Large-scale electronic structure theory provides potential energy surfaces and force fields for simulating complex chemical processes. These processes are important for technology and biological chemistry. A research team led by Donald Truhlar and Osanna Tishchenko of the University of Minnesota uses ALCF resources to obtain accurate energies and stationary points for systems whose electronic structure has high multi-reference character. The researchers employ multi-reference perturbation theory and multi-configuration quasi-degenerate perturbation theory to study three classes of reactive systems in the gas phase and materials.

The computer-intensive part of this research consists of electronic structure calculations required for structural characterization and rate-constant and dynamics calculations. The main software packages for this project are the GAMESS, POLYRATE, and GPAW codes. Computational parallelism is exploited both in the electronic structure and dynamics steps.

The team's work promises to build greater understanding of charge transfer and polarity in molecular electronics; help develop clean, efficient fuels; and advance the science of atmospheric chemistry.

Contact: truhlar@umn.edu, tishc002@umn.edu



A metallofullerene molecule. Sixty carbon atoms combine to form a soccer ball shape, or buckyball. Inside the ball is a single atom of calcium (purple). An electron can transfer to and from the calcium atom to the outer ring structure of the ball.

Image Credit: Osanna Tishchenko and Donald Truhlar, University of Minnesota.

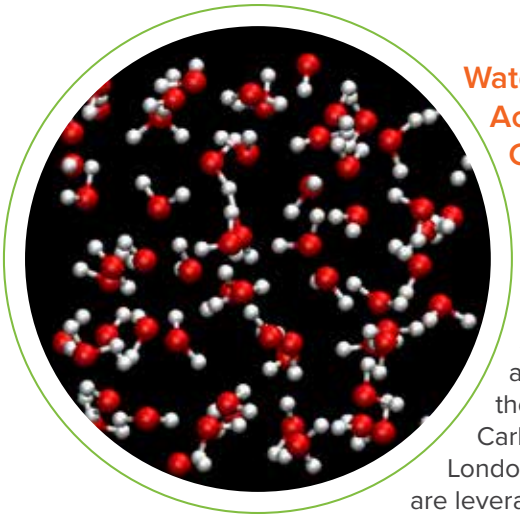
PI: Dario Alfè

INSTITUTION: University College London

ALLOCATION PROGRAM: DD 2012

ALLOCATION HOURS: 1 Million Core-Hours

RESEARCH DOMAIN: Chemistry



Snapshot from a liquid-water DFT simulation at room temperature. QMC energies on such a system have only become possible recently on leadership-class machines like Intrepid and Mira. This image was generated via a DFT simulation on the Cray XT6 HECToR in the U.K.

Image Credit: Dario Alfè, Michael Gillan, and Michael Towler, University College London.

Water Systems from Highly Accurate Quantum Monte Carlo Calculations

Essential to life on earth, water is one of the most familiar substances still not fully understood by modern science. Using the highly accurate electronic structure theory method Quantum Monte Carlo (QMC), University College London researchers led by Dario Alfè are leveraging ALCF resources to model liquid water with unprecedented accuracy. Their efforts will yield fundamental insights applicable in aqueous chemistry across scientific disciplines.

Alfè's team recently coupled QMC with density functional theory (DFT)-based molecular dynamics within their CASINO program, allowing them to calculate the accurate QMC energy of a system on a dynamical trajectory generated using the less expensive DFT calculations. This constitutes the team's first step toward the challenging goal of simulating liquid water with QMC, a material notoriously difficult to account for with DFT. QMC will yield highly accurate results for all the occurring interactions, including the ubiquitous hydrogen bonds.

Contact: d.alfe@ucl.ac.uk

PI: Maya Gokhale

INSTITUTION: Lawrence Livermore National Laboratory

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 10 Million Core-Hours

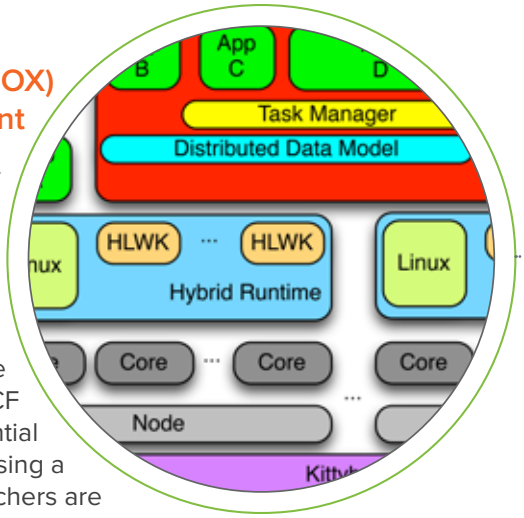
RESEARCH DOMAIN: Computer Science

Fault-Oblivious Exascale (FOX) Computing Environment

As computer speed and power continue to increase, exascale systems—machines with 100 million cores—will someday become the norm. A research team led by Maya Gokhale of the Lawrence Livermore National Laboratory is using ALCF resources to study the potential issues facing these systems. Using a Fault-Oblivious model, researchers are studying fault management by building a software stack and (since exascale machines do not yet exist) using Argonne's petascale systems to test it.

The team is exploring fault isolation and recovery across the entire stack from the operating system, through the runtime, up into the application. The core of this approach is based on a fault-tolerant distributed data store, and a task management system built on top of that. This research is expected to create new applications environments and results from software and library development that can be used to guide the development of future exascale systems.

Contact: gokhale2@llnl.gov



Developing and testing future applications and operating systems for exascale.

Image Credit: Maya Gokhale, Lawrence Livermore National Laboratory.

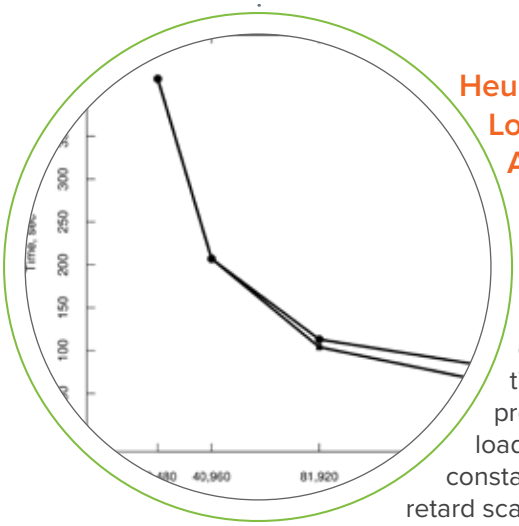
PI: Yuri Alexeev

INSTITUTION: Argonne National Laboratory

ALLOCATION PROGRAM: DD 2012

ALLOCATION HOURS: 1 Million Core-Hours

RESEARCH DOMAIN: Computer Science



Ideal and observed scalability curves based on wall-clock time for the first FMO SCC iteration on Intrepid for 17,767 atoms protein-ligand bio-system.

Image Credit: Yuri Alexeev, Argonne National Laboratory.

Heuristic Static Load-Balancing Algorithm

In petascale supercomputing, load balancing has become critically important. According to Amdahl's law, the scalable component of the total wall time shrinks as the numbers of processors increase, while the load imbalance—together with the constant sequential component—acts to retard scalability. Improved load balancing can be a simple, effective way to boost the scalability and performance of parallel algorithms.

Load balancing is especially important for large systems when the number of tasks is less than or equal to the number of nodes, and/or the tasks have uneven sizes. A research team led by Yuri Alexeev of Argonne National Laboratory is using ALCF resources to develop a heuristic static load-balancing algorithm (HSLB). On 163,840 cores of the IBM Blue Gene/P, the team achieved a parallel efficiency of 80% for computing energy of the 17,767 atoms protein-ligand bio-system by using the Fragment Molecular Orbital (FMO) method implemented in the quantum chemistry package, GAMESS. HSLB has been also successfully applied in the climate-modeling package, CESM.

Contact: yuri@alcf.anl.gov

PI: Ewing Lusk

INSTITUTION: Argonne National Laboratory

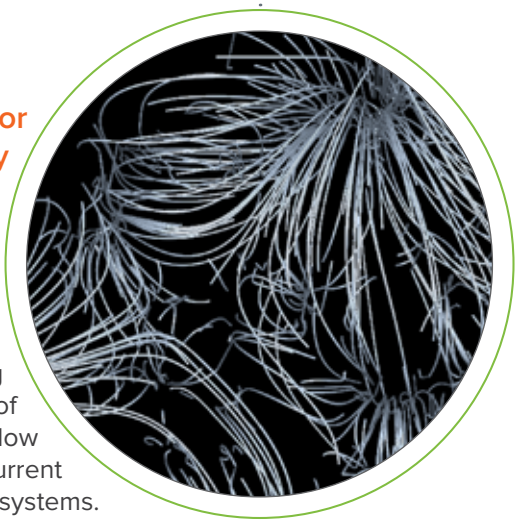
ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 5 Million Core-Hours

RESEARCH DOMAIN: Computer Science

Scalable System Software for Performance and Productivity

System software is a critical component of any computing system and forms the infrastructure on which all applications depend. Using ALCF resources, a research team led by Ewing Lusk is improving and extending the capabilities of existing system software to allow applications to benefit from current leadership-class systems.



Streamlines from an early time step of the Rayleigh-Taylor instability depend on scalable storage, communication, and data analysis algorithms developed at extreme scale using INCITE resources.

Image Credit:
Tom Peterka, Argonne National Laboratory.

As hardware complexity skyrockets in leadership-class systems, it is not easy for applications to take complete advantage of the available system resources and to avoid bottlenecks. This INCITE project aims to improve the performance and productivity of key system software components on these platforms. The research team is studying four classes of system software, using the IBM Blue Gene/P platform to understand and solve problems that occur at scale. Through rigorous experimentation, analysis, and design cycles, the team is improving the capabilities not only of systems being deployed in the near term, but of all systems pushing scalability limits in the near future.

Contact: lusk@mcs.anl.gov

PI: Warren Washington

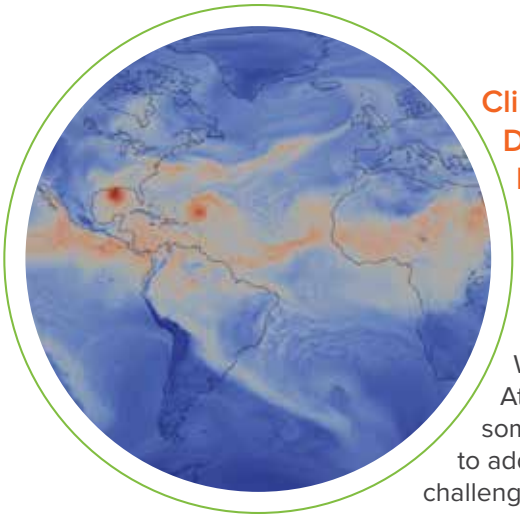
INSTITUTION: National Center for Atmospheric Research

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 86 Million Core-Hours

ALCF: 30 Million; **OLCF:** 56 Million

RESEARCH DOMAIN: Earth Science



A snapshot of the Community Atmosphere Model (CAM5) with spectral element dynamics at 1/8 degree resolution.

Image Credit: Joseph A. Insley, Robert Jacob, and Sheri Mickelson, Argonne National Laboratory; Andy Bauer, Kitware; Mark Taylor, Sandia National Laboratory.

Climate-Science Computational Development Team: The Climate End Station II

Climate-science modeling data helps energy policymakers evaluate and implement changes in national and international policies that affect the global economy. A team led by Warren Washington of the National Center for Atmospheric Research (NCAR) helps coordinate some of the high-performance computing needed to address the world's most significant climate challenges.

The team, comprising scientists from many U.S. Department of Energy (DOE) laboratories and NCAR, conducts simulations that address predictive capability and reduce scientific uncertainties. Simulation data is provided to the world's climate change community through the DOE's Earth System Grid.

The DOE program primarily credited with providing high-resolution model components is Climate Science for a Sustainable Energy Future (CSSEF), coordinated among several DOE laboratories. Together with the Community Earth System Model (CESM) program, their experiments require the thousands of computational cores offered through INCITE.

Scientists design, test, validate, and install important physical model components into the CESM and CSSEF efforts. These components improve the simulations' fidelity and accuracy and are used to perform ensemble simulations for statistically significant projections of potential climate changes worldwide.

Contact: wmw@ucar.edu

PI: Thomas Jordan

INSTITUTION: University of Southern California

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 40 Million Core-Hours

ALCF: 2 Million; **OLCF:** 38 Million

RESEARCH DOMAIN: Earth Science

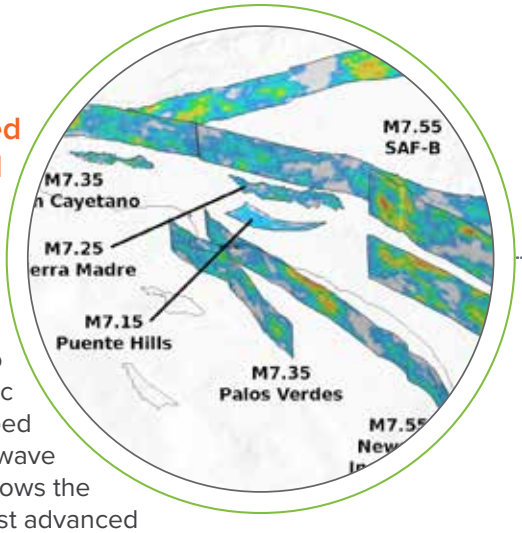
CyberShake 3.0: Physics-Based Probabilistic Seismic Hazard Analysis

A team led by Thomas Jordan of the Southern California Earthquake Center (SCEC) at the University of Southern California is using INCITE to calculate a physics-based probabilistic seismic hazard map for California. Dubbed "CyberShake 3.0," this first-ever 3D wave propagation computational approach shows the seismic hazard implications of the most advanced earthquake forecasts of the U.S. Geological Survey, which produces the nation's official seismic hazard forecasts.

CyberShake 3.0 improves on existing models by better capturing the impact of rupture directivity and sedimentary basin structures on earthquake peak ground motions. In addition, CyberShake introduces never-before-available seismic hazard data products including an extended earthquake rupture forecast and shaking duration forecasts. CyberShake 3.0 represents a pioneering effort to use high-performance computing to improve the broadest-impact seismic hazard data products.

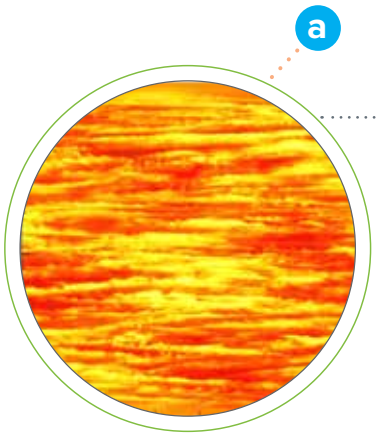
While CyberShake research focuses on the well-studied, seismically vulnerable region of California, the technique is applicable to any seismically active region in the world.

Contact: tjordan@usc.edu



A 3D view showing potential source faults for Southern California's next "big one." Dynamic rupture and wave propagation simulations produce a model of ground motion at the earth's surface. Colors indicate possible distributions of displacement across the faults during rupture.

Image Credit: Geoffrey Ely, Southern California Earthquake Center.



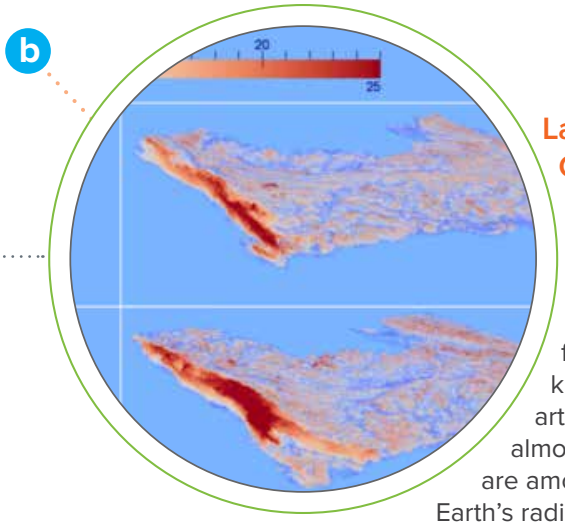
PI: Roberto Paoli

INSTITUTION: CERFACS

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 20 Million Core-Hours

RESEARCH DOMAIN: Earth Science



a) Potential temperature fluctuations of the atmosphere in a vertical plane in the middle of the computational domain. b) 3D snapshots of ice mixing ratio.

Image Credit: Roberto Paoli and Odile Thouron, CERFACS.

Large Eddy Simulations of Contrail-to-Cirrus Transition

Contrails are ice clouds that form by condensed water-vapor exhaust from aircraft engines. When contrails spread to form cirrus clouds, they can persist for hours, extending over several square kilometers. These "contrail cirrus," which artificially increase cloudiness and become almost indistinguishable from natural cirrus, are among the most uncertain contributors to Earth's radiative forcing. And as demand for air travel grows, contrail cirrus represents increasing concern for scientists and policymakers.

Roberto Paoli from CERFACS leads a research team studying the contrail-to-cirrus transition through simulations with the atmospheric solver Meso-NH. Using ALCF resources, they identified the key processes that determine the dynamical and microphysical characteristics of the contrail as a function of age. Their simulations—the largest ever performed in this area to date—found that ambient turbulence controls the initial contrail evolution whereas radiative transfer is the main driver later. Radiative transfer produces regions of local cooling and heating inside the cloud, tending to redistribute ice along a single vertical layer and forming the characteristic puffy structures of natural cirrus.

Contact: paoli@cerfacs.fr

PI: Greg Holland

INSTITUTION: National Center for Atmospheric Research

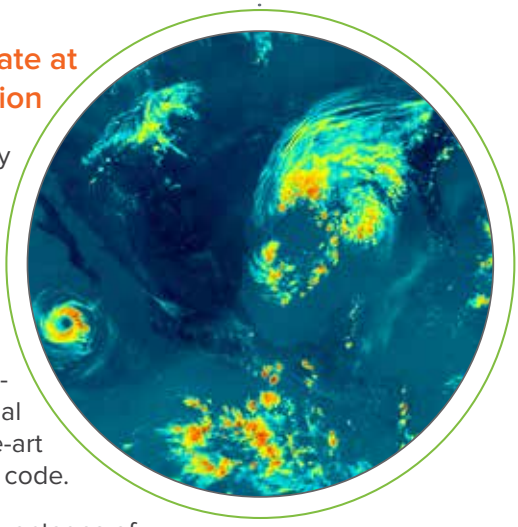
ALLOCATION PROGRAM: ALCC 2011-2012

ALLOCATION HOURS: 13 Million Core-Hours

RESEARCH DOMAIN: Earth Science

Simulating Regional Climate at Convection Permitting Resolution

Using ALCF resources, a team led by Greg Holland of the National Center for Atmospheric Research (NCAR) is working to create next-generation climate modeling systems that may ultimately aid in national planning for extreme weather events. The team has completed the longest, highest-resolution run of the Nested Regional Climate Model (NRCM), a state-of-the-art climate modeling code.



Color-enhanced satellite view snapshot from a recent climate simulation using the Nested Regional Climate Model at 4 kilometers horizontal resolution.

Image Credit: James Done, National Center for Atmospheric Research (NCAR) Earth System Laboratory.

The study examines the advantages of convection-permitting resolution on climate timescales with an emphasis on high-impact weather and climate. In a breakthrough for climate simulations, this project has run NRCM at a horizontal resolution of 4 kilometers for a large domain extending over North America and the Atlantic Ocean basin.

Analysis is now underway on phenomena with high sensitivity to model resolution, including water-snowpack assessments and such high-impact events as winter storms and hurricanes. The research promises to advance understanding of Earth's climate for national emergency preparedness and will broaden the community of researchers capable of using leadership computing resources.

Contact: gholland@ucar.edu

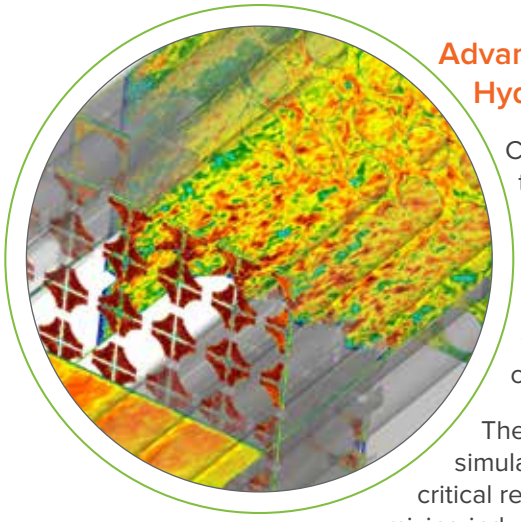
PI: Paul F. Fischer

INSTITUTION: Argonne National Laboratory

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 25 Million Core-Hours

RESEARCH DOMAIN: Energy Technologies



Velocity magnitude distribution in a flow through the 25-pin swirl-vane spacer grid of the Matis benchmark. Computed on Intrepid with Nek5000 and visualized on Eureka with VisIt at the ALCF.

Image Credit: Paul F. Fischer, Aleks Obabko, and Tim Tautges, Argonne National Laboratory.

Advanced Reactor Thermal Hydraulic Modeling

Clean, safe nuclear power is essential for the world's growing energy needs. A team led by Paul Fischer and Aleksandr Obabko of Argonne National Laboratory uses ALCF resources to perform highly accurate computations that allow them to analyze, model, simulate, and predict complex thermo-fluid phenomena.

The team carried out large-scale numerical simulations of turbulent thermal transport in critical reactor components. Researchers analyzed mixing induced by wire-wrap spacers for 7-, 19-, 37-, and 217-pin subassemblies and spacer-grid mixing for a 5x5 subassembly. The latter analysis was submitted as part of a NEA/OECD benchmark study that ranked in the top submissions for mean and rms velocity predictions. In another NEA/OECD benchmark problem, the team ranked first in prediction of thermal striping—alternating hot and cold patches—induced when streams of different temperatures mix at a T-junction.

Their current computations are some of the largest to date with the spectral element code Nek5000, and involve several hundred million grid points on unstructured meshes.

The team's findings are expected to inform the design of next-generation nuclear reactors capable of providing sustainable energy with a low carbon footprint.

Contact: fischer@mcs.anl.gov

PI: Mihai Anitescu

INSTITUTION: Argonne National Laboratory

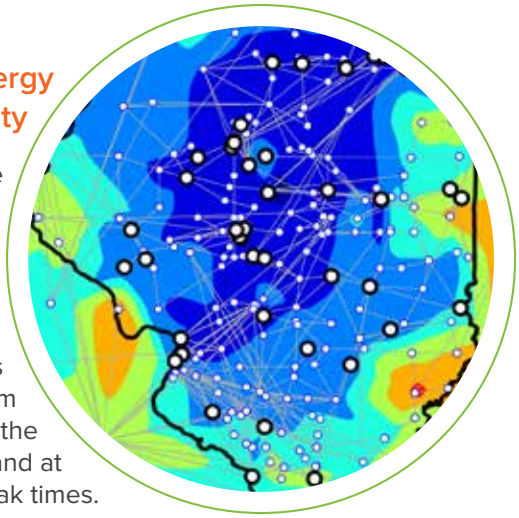
ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 10 Million Core-Hours

RESEARCH DOMAIN: Energy Technologies

Optimization of Complex Energy System Under Uncertainty

The federal mandate to increase the use of renewable energy has resulted in a significant challenge for the U.S. power grid. Unlike fossil-fuel generation systems, the available amount of renewable energy at any given time is uncertain. As a result, a system relying on renewable energy runs the risk of not meeting consumer demand at peak times.



The Illinois power grid system is overlaid on fields portraying electricity prices under a deterministic economic dispatch scenario. Dark-blue areas have the lowest prices while red and yellow have the highest. Argonne researchers use a model of the Illinois grid to test algorithms for making power dispatch decisions under uncertainty.

Image Credit:
Mihai Anitescu, Argonne National Laboratory.

A team of scientists led by Mihai Anitescu of Argonne National Laboratory is using high-performance computing to explore optimization under uncertainty as the paradigm for managing uncertainty in the renewable energy supply. Their goal is to reduce reserve requirements and stabilize electricity markets in the next-generation power grid. The team uses stochastic programming formulations of the decision process that schedules supply and matches demand.

To date, the team has demonstrated that, at least on some configurations, even 20% wind penetration—the federal mandate for the year 2030—can be accommodated without significant reserve increase by using stochastic optimization, a result that would not be achievable with traditional formulations.

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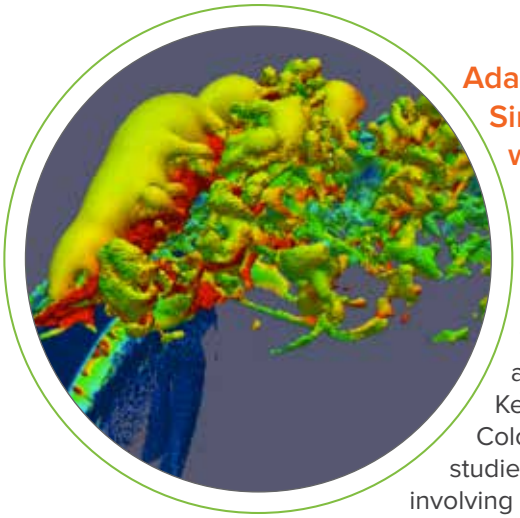
PI: Kenneth Jansen

INSTITUTION: University of Colorado

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 40 Million Core-Hours

RESEARCH DOMAIN: Engineering



A snapshot of a simulation showing synthetic jet geometry and resulting flow isosurface of vertical velocity, colored by total speed.

Image Credit: Michel Rasquin, University of Colorado.

Adaptive Detached Eddy Simulation of a Vertical Tail with Active Flow Control

With fuel being the airline industry's single largest expense, fuel economy is a top priority. A key to reducing fuel consumption is reducing the weight of the aircraft. A research team led by Kenneth Jansen of the University of Colorado is conducting flow control studies for innovations in lighter designs involving the wings and vertical tail of the aircraft.

To take off or land, aircraft rely on mechanical wing flaps to provide additional lift. The flaps serve no in-flight purpose and their weight reduces the plane's fuel efficiency. Researchers are performing a series of simulations of active flow control using high-frequency jets known as "synthetic jets" with smaller, lighter mechanical flaps.

Using the synthetic jets, the team is also conducting simulations of active flow control on the vertical tail of the aircraft. Researchers hypothesize that such design modifications could reduce fuel use by 0.5%, resulting in annual savings of $300 million.

Contact: jansenke@colorado.edu

PI: Elia Merzari

INSTITUTION: Argonne National Laboratory

ALLOCATION PROGRAM: ALCC 2012-2013

ALLOCATION HOURS: 30 Million Core-Hours

RESEARCH DOMAIN: Engineering

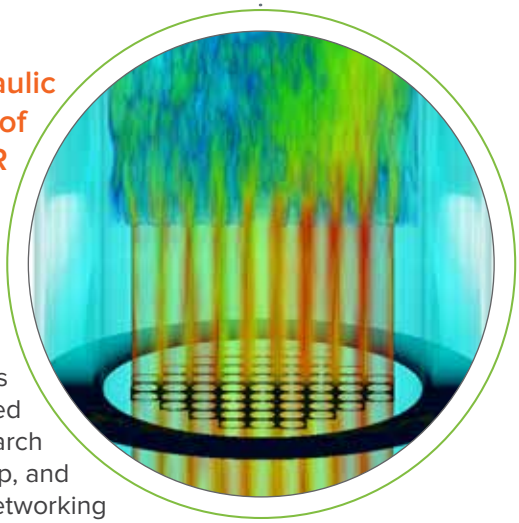
Petascale Thermal-Hydraulic Simulations in Support of CESAR

The Center for Exascale Simulation for Advanced Reactors (CESAR) aims to develop a coupled next-generation nuclear reactor core simulation tool for exascale computing platforms. CESAR helps fulfill the mission of the Advanced Scientific Computing Research program: to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the U.S. Department of Energy.

A team led by Elia Merzari of Argonne National Laboratory is using ALCF resources to create extreme-fidelity physics models that will enable new reactor design analysis in existing and next-generation reactors on exascale computing platforms.

The team's simulations address the limitations of current methods as well as potential scaling to larger machines. Data from one simulation is expected to provide insight into the challenges of exascale simulations. Data from another simulation—a full high-fidelity large eddy simulation of a 37-rod bundle—will be used to examine rod-bundle flows at a level never achieved before, helping to determine computational cost in the exascale limit.

Contact: emerzari@anl.gov



This snapshot of a numerical simulation of the MASLWR experiment shows a cross-section with view of the velocity magnitude.

Image Credit:
Elia Merzari, Argonne National Laboratory.

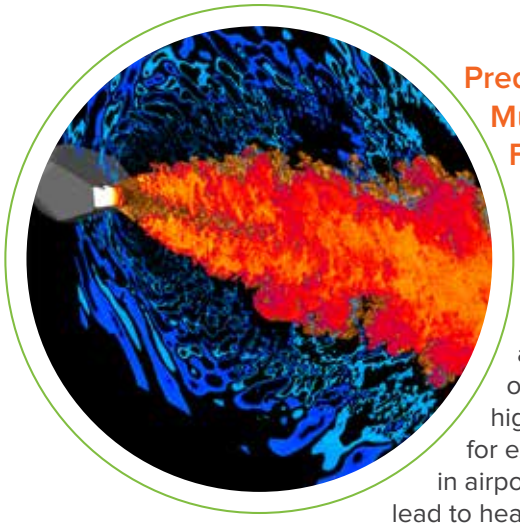
PI: Parviz Moin

INSTITUTION: Center for Turbulence Research, Stanford University

ALLOCATION PROGRAM: ALCC 2012-2013

ALLOCATION HOURS: 80 Million Core-Hours

RESEARCH DOMAIN: Engineering



The rectangular nozzle is shown in gray with an isosurface of temperature (gold) cut along the center plane of the nozzle showing temperature contours (red/yellow). The acoustic field is visualized by (blue/cyan) contours of the pressure field taken along the same plane. The chevrons enhance turbulent mixing just downstream of the nozzle exit shaping how the jet spreads downstream. This significantly reduces the noise produced by the supersonic jet compared to a rectangular nozzle without chevrons (not shown).

Image Credit: Joseph Nichols, Center for Turbulence Research.

Prediction of Multiscale, Multiphysics Turbulent Flow Phenomena Using Unstructured Large Eddy Simulation

Engine exhaust noise—particularly during take-off and landing approaches—represents a major obstacle to the widespread use of high-speed aircraft. Supersonic jets, for example, raise noise pollution levels in airport communities and can ultimately lead to hearing loss for crew on aircraft carrier decks. A team led by Parviz Moin of Stanford University's Center for Turbulence Research is using the power of supercomputers at the ALCF to study supersonic jet noise.

For reasons as yet not completely understood, serrated engine exhaust nozzles are known to reduce noise, and in particular eliminate "crackle," an especially noxious component of the noise. Such serrations, called chevrons, are featured on Boeing's new 787 aircraft. The research team is performing simulations to determine how and why the chevrons work. This comprehensive study relies on one-of-a-kind large eddy simulations of supersonic jet noise involving complex nozzle geometries.

This project is supported by the U.S. Air Force Office of Scientific Research and the U.S. Naval Air Systems Command.

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PI: Subramanian Sankaranarayanan

INSTITUTION: Argonne National Laboratory

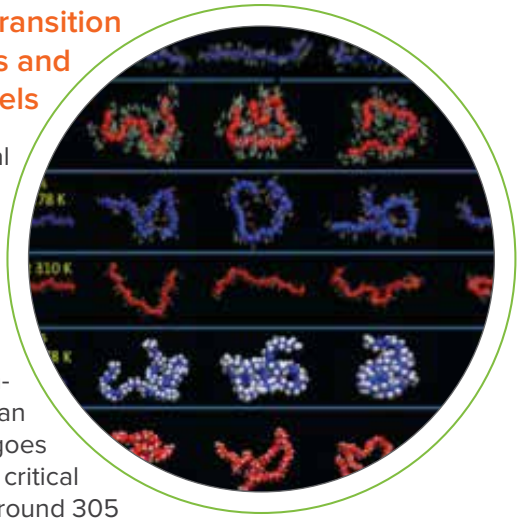
ALLOCATION PROGRAM: ALCC 2012-2013

ALLOCATION HOURS: 50 Million Core-Hours

RESEARCH DOMAIN: Materials Science

Dynamics of Conformational Transition in Thermo-Sensitive Polymers and Hydrogels

Understanding the conformational changes in isolated linear polymer chains and their macromolecular architectures is a fundamental problem in polymer science. External stimuli and alterations in environmental variables can bring about these changes. Thermo-sensitive polymers such as poly(n-isopropylacrylamide) (PNIPAM) represent an important class of materials that undergoes coil-to-globule transition across the lower critical solution temperature (LCST), which is around 305 degrees Kelvin.



Conformational dynamics in singe chain thermosensitive polymers and their macroscopic architectures.

Image Credit: Subramanian Sankaranarayanan, Argonne National Laboratory.

A team led by Subramanian Sankaranarayanan at Argonne National Laboratory's Center for Nanoscale Materials is using ALCF resources to study conformational transitions in thermo-sensitive oligomers and their macroscopic architectures such as polymer brushers and polymer gels. Coil-to-globule transitions are of importance in a number of practical applications, including drug delivery, medical diagnostics, tissue engineering, electrophoresis, separation, and enhanced oil recovery. For example, tuning the LCST of PNIPAM close to human body temperature via copolymerization can enable development of a controlled drug delivery system. The team's work will extend to macromolecular architectures such as polymer brushes and gels of PNIPAM.

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PIs: Priya Vashishta, Aiichiro Nakano

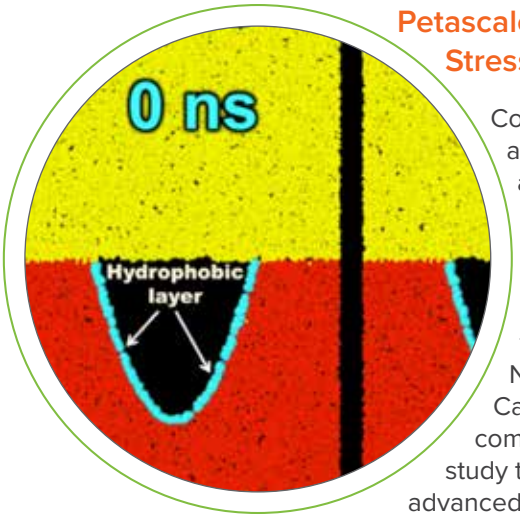
INSTITUTION: University of Southern California

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 45 Million Core-Hours

RESEARCH DOMAIN: Materials Science

Petascale Simulations of Stress Corrosion Cracking



A snapshot of the central slice of the silica-water system with a hydrophobic layer on the cavity surface. Silica is shown in red, the water layer in yellow, and the hydrophobic layer is shown in blue dots.

Image Credit: Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta, and Adarsh Shekhar, Collaboratory for Advanced Computing and Simulations, University of Southern California.

Corrosion is a complex technological and economic problem that imposes an annual cost of about 3% of the U.S. gross domestic product. Stress-induced corrosion limits the performance and lifetime of materials used in energy and nuclear technologies. A research team led by Priya Vashishta and Aiichiro Nakano of the University of Southern California is using the high-performance computing capabilities of the ALCF to study this corrosion in nickel-based alloys in advanced nuclear reactors and in glass containers of nuclear waste.

The team is performing molecular dynamics and quantum mechanical simulations to understand the atomistic mechanisms that control stress corrosion cracking. These simulations allow the team to investigate how even a small amount of sulfur impurity in nickel-based alloys and water in silicate glass can initiate material damage resulting in fracture.

Their findings promise to advance the understanding of the complex electrochemical processes that lead to stress corrosion cracking and, ultimately, the development of new technologies to prevent it.

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PI: James R. Chelikowsky

INSTITUTION: The University of Texas at Austin

ALLOCATION PROGRAM: ALCC 2011-2012

ALLOCATION HOURS: 12 Million Core-Hours

RESEARCH DOMAIN: Materials Science

Toward Crystal Engineering from First Principles

Crystal engineering is a bottom-up approach to designing new crystalline materials from molecular building blocks with vast and far-reaching applications, from drug design to hydrogen storage. Researchers James Chelikowsky and Noa Marom of The University of Texas at Austin, in collaboration with Alexandre Tkatchenko from the Fritz Haber Institute of the Max Planck Society in Berlin are using ALCF resources to study the intermolecular dispersion interactions that govern structure and properties of molecular crystals. The team's goal is to enable computational crystal engineering from first principles. To this end, density functional theory (DFT) is employed in conjunction with a newly developed methods for describing many-body dispersion (MBD) interactions.

The research focuses primarily on demonstrating the capability of the DFT+MBD approach for a series of case studies reflecting the wide variety of applications of crystal engineering from biological systems, such as amino acids and antimalarial drugs, to technological applications, such as organic semiconductors for organic electronics and dye-sensitized TiO_2 clusters for solar cells. The systems being studied comprise several hundred atoms, pushing the size limits of fully quantum mechanical calculations. Potential energy surface (PES) exploration for such systems requires massively parallel computing. Accounting for MBD interactions is crucial for locating the PES minima for molecular crystals. In the figure this is illustrated for PES projections on to the *a-b* plane of the γ-glycine crystal.

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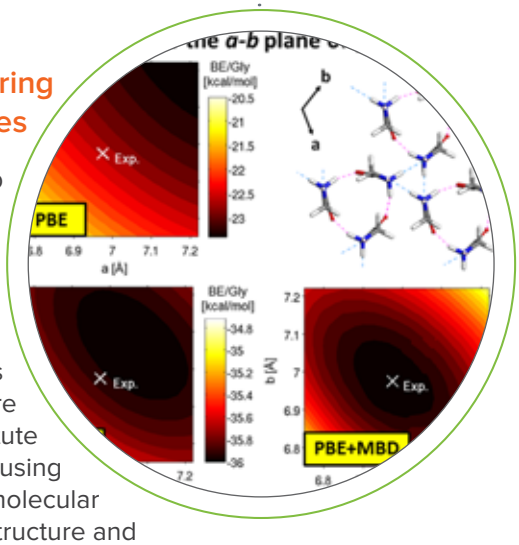


This partial image shows the potential energy surface projected on to the a-b plane of the γ-glycine crystal (illustrated on the top right) calculated using DFT without any dispersion method (top left), DFT with the TS dispersion method (bottom left), and DFT with the MBD dispersion method (bottom right). Only the latter is in agreement with experiment.

Image Credit:
James Chelikowsky and Noa Marom, The University of Texas at Austin; Viktor Atalla, Sergey Levchenko, Anthony M. Reilly, and Alexandre Tkatchenko, Fritz Haber Institute; Robert A. DiStasio Jr., Princeton University; Leslie Leiserowitz, Weizmann Institute of Science.

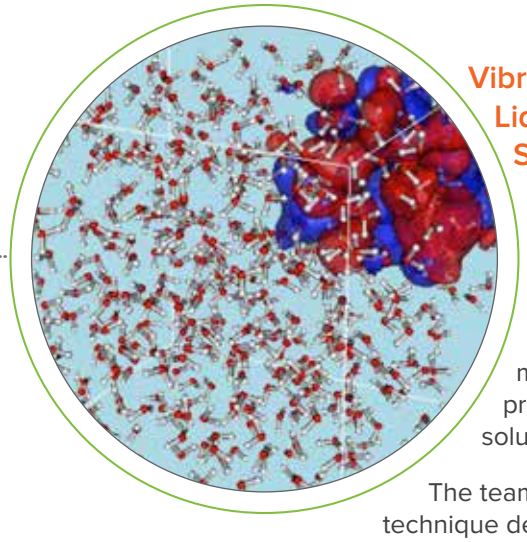
PI: Giulia Galli

INSTITUTION: University of California, Davis

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 25 Million Core-Hours

RESEARCH DOMAIN: Materials Science



Isosurfaces of a molecular orbital in a 512-molecule water sample. The orbital is localized to an octant of the simulation cell as a result of the application of the recursive bisection algorithm. This localization property is then used to accelerate the computation of the exchange energy.

Image Credit: Francois Gygi, University of California, Davis.

Vibrational Spectroscopy of Liquid Mixtures and Solid-Liquid Interfaces

Aqueous solutions of simple salts are of great interest in electrochemistry and atmospheric chemistry. A research team led by Giulia Galli at the University of California, Davis uses first-principles molecular dynamics (MD) simulations to predict the properties of simple aqueous solutions and interpret spectroscopic data.

The team is using the Qbox code and a bisection technique developed by Francois Gygi to compute the Hartree-Fock exchange energy, greatly increasing the efficiency of ab initio simulations with hybrid functionals.

The bisection method allows for an unbiased localization of orbitals in domains of varying size and a truncation of orbitals that preserves accuracy in a controlled manner. The method targets large-scale parallel computers and relies on a parallel Jacobi algorithm for simultaneous diagonalization and a systolic algorithm for the computation of exchange integrals. Scalability on up to 16k cores of the ALCF Mira platform was demonstrated for a system of 256 water molecules. The method is particularly well adapted to study inhomogeneous systems such as solid-liquid interfaces and solvated nanoparticles, in which molecular orbitals do not exhibit simple localization patterns.

Work is in progress to simulate realistic models of solid-liquid interfaces relevant to atomic-scale phenomena in photo-electrochemical cells and batteries.

Contact: gagalli@ucdavis.edu

PI: Paul Mackenzie

INSTITUTION: Fermi National Accelerator Laboratory

ALLOCATION PROGRAM: INCITE 2012

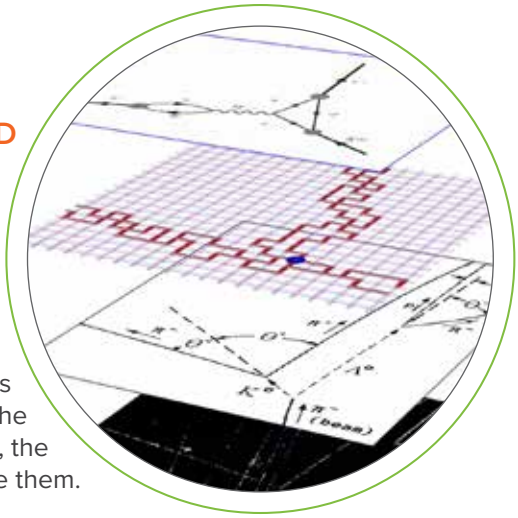
ALLOCATION HOURS: 96 Million Core-Hours

ALCF: 50 Million; **OLCF:** 46 Million

RESEARCH DOMAIN: Physics

Lattice QCD

Quantum chromodynamics (QCD) research plays a key role in the ongoing efforts of scientists to develop a unified theory of the fundamental forces of nature. While scientists understand the behavior of such atomic particles as protons and neutrons, less is known about the interactions of quarks and gluons, the subatomic particles that comprise them.



This diagram illustrates the wide range of distance scales that must be understood before the calculations of the decay of a kaon into two pions can be performed.

Image Credit: Norman Christ, Columbia University; RBC/USQCD collaboration.

Using the capabilities of the ALCF's Blue Gene/P supercomputer, the United States Quantum Chromodynamics (USQCD) Collaboration carries out extensive calculations on lattice gauge theory, the theory that describes how quarks and gluons help form atomic nuclei. Paul Mackenzie of the Fermi National Accelerator Laboratory leads the USQCD team.

The USQCD efforts lie at the heart of the U.S. Department of Energy's large experimental programs in high energy and nuclear physics.

Contact: mackenzie@fnal.gov

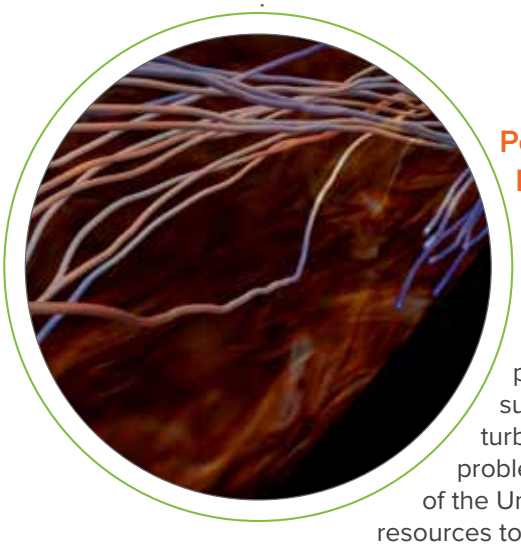
PI: Jean C. Perez

INSTITUTION: University of New Hampshire

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 10 Million Core-Hours

RESEARCH DOMAIN: Physics



A snapshot of turbulent magnetic field lines inside a coronal hole that expands from a small patch on the solar surface to five solar radii.

Image Credit: Jean C. Perez, University of New Hampshire.

Petascale Simulations of Inhomogeneous Alfvén Turbulence in the Solar Wind

The origin of the solar wind and the heating of the solar corona are two of the most compelling problems in heliospheric physics. In-situ and remote observations suggest that Alfvén waves (AWs) and AW turbulence play a key role in solving both problems. A research team led by Jean Perez of the University of New Hampshire is using ALCF resources to address these issues and arrive at new theoretical understandings.

Scientists are conducting the first direct numerical simulations of AW turbulence in the extended solar atmosphere that account for the inhomogeneities in the density, flow speed, and background magnetic field within a narrow magnetic flux tube extending from roughly one solar radius to eleven solar radii. They are comparing their numerical simulations with remote observations. Researchers are using the Inhomogeneous Reduced Magnetohydrodynamics Code developed by Perez and extensively tested and benchmarked on the IBM Blue Gene/P.

This study is of added interest to the space physics community, given preparations underway for NASA's Solar Probe Plus mission with its planned 2018 launch date.

Contact: jeanc.perez@unh.edu

PI: Sean Couch

INSTITUTION: The University of Chicago

ALLOCATION PROGRAM: DD 2012

ALLOCATION HOURS: 5 Million Core-Hours

RESEARCH DOMAIN: Physics

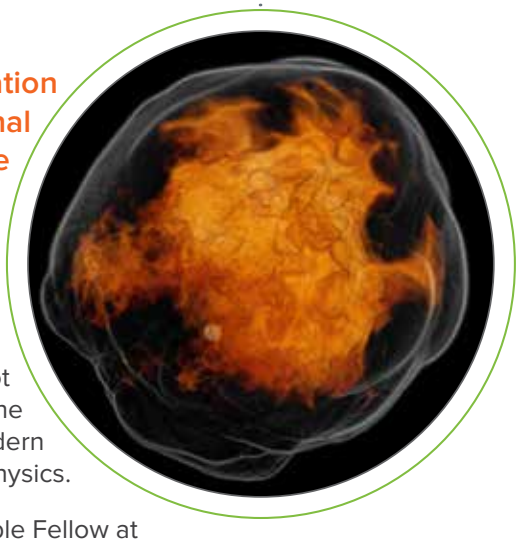
Petascale Simulation of Magnetorotational Core-Collapse Supernovae

Core-collapse supernovae are the luminous explosions that herald the death of massive stars. While its importance in galactic evolution cannot be underestimated, the core-collapse supernova mechanism is not fully understood and remains one of the most important challenges for modern computational astrophysics.

A research team led by Sean Couch, Hubble Fellow at the University of Chicago, is using ALCF resources to conduct first-ever simulations to explore the influence of magnetic fields and rotation on the mechanisms that reverse stellar core collapse and drive a supernova. These simulations allow researchers to predict the spins, kicks, magnetic field strengths, and alignments of newly formed neutron stars, pulsars, and magnetars as well as the dependence of these parameters on originating conditions.

Recent findings show substantial differences in the behavior of 2D and 3D buoyant plumes, suggesting that 3D characteristics are necessary for realistic simulations. These groundbreaking studies may profoundly expand our understanding of stellar death and the creation of heavy elements throughout the universe.

Contact: smc@flash.uchicago.edu



Volume rendering of the highest entropy plumes in a 3D core-collapse supernova simulation. The edge of the nascent neutron star is shown as the faint blue sphere near the center. Entropy, a measure of the thermodynamic disorder, shows the buoyant convective plumes and turbulence that play a critical part in the core-collapse supernova mechanism. The surface of the outgoing shock wave is also shown in faint gray.

Image Credit: Sean Couch, The University of Chicago.

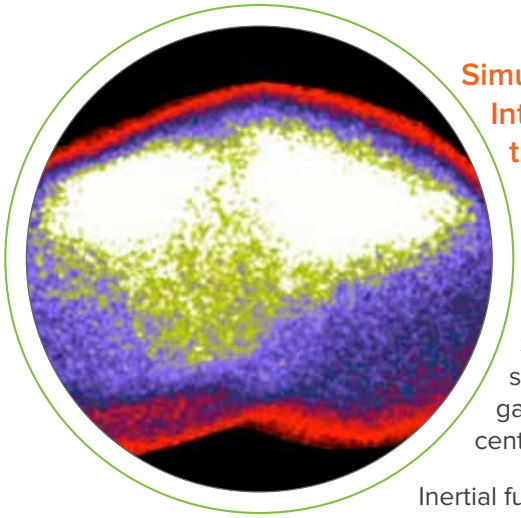
PI: Denise Hinkel

INSTITUTION: Lawrence Livermore National Laboratory

ALLOCATION PROGRAM: INCITE 2012

ALLOCATION HOURS: 63 Million Core-Hours

RESEARCH DOMAIN: Physics



Laser input to a pF3D simulation of two NIF laser quads propagating through an ignition target. Here, power transferred from other quads of laser beams is distributed uniformly across the laser beams. Two quads overlap in the simulated region. This enhances reflectivity through a shared reflected light wave.

Image Credit: Denise Hinkel, Bruce Langdon, Steven Langer, Charles Still, and Edward Williams, Lawrence Livermore National Laboratory.

Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond

Providing for the world's energy demands is one of the most urgent and difficult challenges facing society. Scientists have been working to achieve self-sustaining nuclear fusion and energy gain in the laboratory for more than a half-century.

Inertial fusion energy provides an attractive solution to the demands for safe, secure, environmentally sustainable energy. To this end, the National Ignition Facility is using the world's most powerful laser to achieve ignition, bringing the goal of fusion energy closer to realization. A key aspect of laser driven fusion is coupling the laser energy to the ignition target. A team of scientists led by Denise Hinkel of Lawrence Livermore National Laboratory is using ALCF resources to perform simulations that provide the details of the coupling process in these ignition targets.

The team's state-of-the-art simulations quantify how overlapping beam quads impact backscatter. These simulations show that overlapping quads can share a reflected light wave, enhancing reflectivity. In a recent simulation, the team saw SBS and SRS backscatter with competition for the incident laser light between them.

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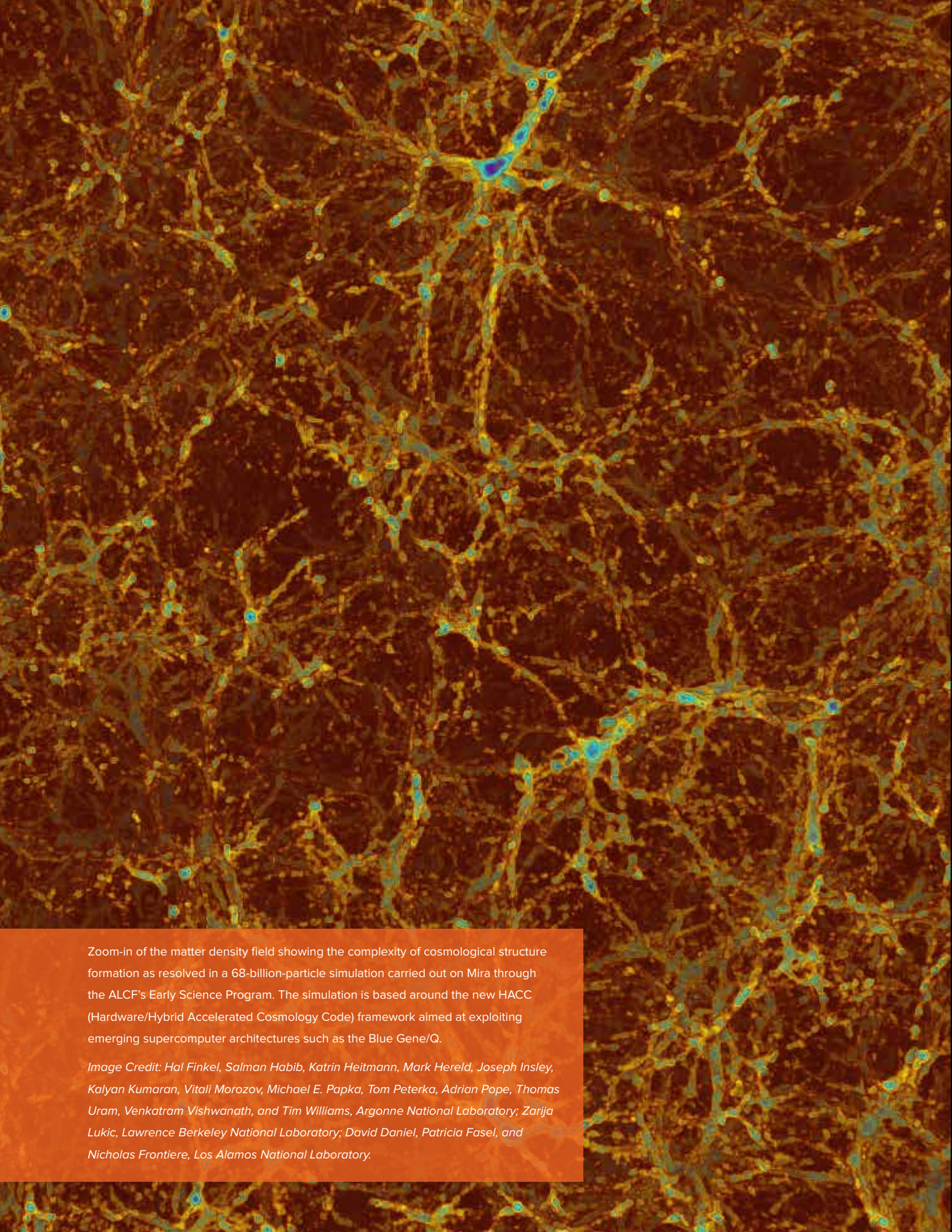

Zoom-in of the matter density field showing the complexity of cosmological structure formation as resolved in a 68-billion-particle simulation carried out on Mira through the ALCF's Early Science Program. The simulation is based around the new HACC (Hardware/Hybrid Accelerated Cosmology Code) framework aimed at exploiting emerging supercomputer architectures such as the Blue Gene/Q.

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

PUBLICATIONS & PROJECTS

2012 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.

This list contains 150 publications in descending order of their publication dates. An asterisk after a name designates an Argonne author. ALCF publications are listed online at http://www.alcf.anl.gov/publications.

Quaglioni, S., Navrátil, P., Hupin, G., Langhammer, J., Romero-Redondo, C., Roth, R., **"No-Core Shell Model Analysis of Light Nuclei,"** *Few-Body Systems*, December 2012, Springer Vienna.

Ray, N., Wang, D., Jiao, X., Glimm, J., **"High-Order Numerical Integration over Discrete Surfaces,"** *SIAM: Society for Industrial and Applied Mathematics*, December 2012, vol. 50, no. 6, pp. 3061-3083.

Leigh, J., Johnson, A., Renambot, L., Vishwanath, V.,* Peterka, T.,* Schwarz, N., **"Visualization of Large-Scale Distributed Data,"** *Data Intensive Distributed Computing: Challenges and Solutions for Large-Scale Information Management*, December 2012, IGI Global.

Maris, P., Aktulga, H.M., Caprio, M.A., Çatalyürek, U.V., Ng, E.G., Oryspayev, D., Potter, H., Saule, E., Sosonkina, M., Vary, J.P., Yang, C., Zhou, Z., **"Large-Scale Ab Initio Configuration Interaction Calculations for Light Nuclei,"** *Journal of Physics: Conference Series*, December 2012, vol. 403, IOP Publishing.

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Caprio, M.A., Maris, P., Vary, J.P., **"The No-Core Shell Model with General Radial Bases,"** *Journal of Physics: Conference Series*, December 2012, vol. 403, IOP Publishing.

Tallent, N., Mellor-Crummey, J., **"Using Sampling to Understand Parallel Program Performance,"** in *Tools for High Performance Computing 2011*, December 2012, Springer-Verlag Berlin, Heidelberg, pp. 13-25.

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Li, L., Larsen, A.H., Romero, N.A.,* Morozov, V.A.,* Glinsvad, C., Abild-Pedersen, F., Greeley, J.,* Jacobsen, K.W., Nørskov, J.K., **"Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters,"** *Journal of Physical Chemistry Letters*, December 2012, vol. 4, no. 1, American Chemical Society, pp. 222-226.

Dubey, A., Daley, C., ZuHone, J., Ricker, P.M., Weide, K., Graziani, C., **"Imposing a Lagrangian Particle Framework on an Eulerian Hydrodynamics Infrastructure in Flash,"** *Astrophysical Journal*, December 2012, vol. 201, no. 2, IOP Publishing.

Higdon, D., Lawrence, E., Heitmann, K.,* Habib, S.,* **"Simulation-Aided Inference in Cosmology,"** in *Statistical Challenges in Modern Astronomy V*, December 2012, SpringerLink, pp. 41-57.

Jiang, W.,* Luo, Y.,* Maragliano, L., Roux, B., **"Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer,"** *Journal of Chemical Theory and Computation*, December 2012, vol. 8, no. 11, American Chemical Society, pp. 4672-4680.

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2012 ALCF PROJECTS

2012 INCITE PROJECTS

Biological Sciences

Protein-Ligand Interaction Simulations and Analysis
T. Andrew Binkowski, Argonne National Laboratory
Allocation: 10 Million Core-Hours

Multiscale Blood Flow Simulations
George Karniadakis, Brown University
Allocation: 73 Million Core-Hours
ALCF: 50 Million; OLCF: 23 Million

Chemistry

Towards Breakthroughs in Protein Structure Calculation and Design
David Baker, University of Washington
Allocation: 33 Million Core-Hours

Simulations of Deflagration-to-Detonation Transition in Reactive Gases
Alexei Khokhlov, The University of Chicago
Allocation: 20 Million Core-Hours

Energetic Aspects of CO_2 Absorption by Ionic Liquids from Quantum Monte Carlo
William Lester, UC Berkeley
Allocation: 4 Million Core-Hours

Large Eddy Simulation of Two-Phase Flow Combustion in Gas Turbines
Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Allocation: 10 Million Core-Hours

Potential Energy Surfaces for Simulating Complex Chemical Processes
Donald Truhlar, University of Minnesota
Allocation: 15 Million Core-Hours

Computer Science

Scalable System Software for Performance and Productivity
Ewing Lusk, Argonne National Laboratory
Allocation: 5 Million Core-Hours

Fault-Oblivious Exascale Computing Environment
Ronald Minnich, Sandia National Laboratories
Allocation: 10 Million Core-Hours

Performance Evaluation and Analysis Consortium End Station
Patrick H. Worley, Oak Ridge National Laboratory
Allocation: 28 Million Core-Hours
ALCF: 10 Million; OLCF: 18 Million

Earth Science

CyberShake 3.0: Physics-Based Probabilistic Seismic Hazard Analysis
Thomas Jordan, Southern California Earthquake Center
Allocation: 40 Million Core-Hours
ALCF: 2 Million; OLCF: 38 Million

Large Eddy Simulations of Contrail-to-Cirrus Transition
Roberto Paoli, CERFACS
Allocation: 20 Million Core-Hours

Climate-Science Computational Development Team: The Climate End Station II
Warren Washington, National Center for Atmospheric Research
Allocation: 86 Million Core-Hours
ALCF: 30 Million; OLCF: 56 Million

Energy Technologies

Optimization of Complex Energy System Under Uncertainty
Mihai Anitescu, Argonne National Laboratory
Allocation: 10 Million Core-Hours

Advanced Reactor Thermal Hydraulic Modeling
Paul Fischer, Argonne National Laboratory
Allocation: 25 Million Core-Hours

Atomistic Adaptive Ensemble Calculations of Eutectics of Molten Salt Mixtures
Saivenkataraman Jayaraman, Sandia National Laboratories
Allocation: 10 Million Core-Hours

Enabling Green Energy and Propulsion Systems via Direct Noise Computation
Umesh Paliath, GE Global Research
Allocation: 45 Million Core-Hours

Engineering

Direct Simulation of Fully Resolved Vaporizing Droplets in a Turbulent Flow
Said Elghobashi, University of California—Irvine
Allocation: 20 Million Core-Hours

Stochastic (w*) Convergence for Turbulent Combustion
James Glimm, Stanford University
Allocation: 35 Million Core-Hours

Adaptive Detached Eddy Simulation of a Vertical Tail with Active Flow Control
Kenneth Jansen, University of Colorado—Boulder
Allocation: 40 Million Core-Hours

Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability
Sanjiva Lele, Stanford University
Allocation: 20 Million Core-Hours

Materials Science

Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces
Giulia Galli, University of California—Davis
Allocation: 25 Million Core-Hours

High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry
William George, National Institute of Standards
Allocation: 22 Million Core-Hours

Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations
Jeffrey Greeley, Argonne National Laboratory
Allocation: 10 Million Core-Hours

Petascale Simulations of Stress Corrosion Cracking
Priya Vashishta, University of Southern California
Allocation: 45 Million Core-Hours

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

Physics

Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond
Denise Hinkel, Lawrence Livermore National Laboratory
Allocation: 63 Million Core-Hours

Toward Exascale Computing of Type Ia and Ib, c Supernovae: V&V of Current Models
Donald Lamb, The University of Chicago
Allocation: 40 Million Core-Hours

Lattice QCD
Paul Mackenzie, Fermi National Accelerator Laboratory
Allocation: 96 Million Core-Hours
ALCF: 50 Million; OLCF: 46 Million

Petascale Simulations of Inhomogeneous Alfvén Turbulence in the Solar Wind
Jean Perez, University of New Hampshire
Allocation: 10 Million Core-Hours

Nuclear Structure and Nuclear Reactions
James Vary, Iowa State University
Allocation: 18 Million Core-Hours

2012 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, The University of Chicago
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

2012 EARLY SCIENCE PROGRAM 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
Benoit Roux, Argonne National Laboratory and 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 Multi-Scale 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, University of Texas
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 & 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

2012 DIRECTOR'S DISCRETIONARY PROJECTS

Biological Science

Multi-Scale Simulations of Deformable Blood Vessels
Leopold Grinberg, Brown University
Allocation: 500,000 Core-Hours

High-Performance Neuron Simulations on the Blue Gene/Q
Michael Hines, Yale University
Allocation: 1 Million Core-Hours

Chemistry

Water Systems from Highly Accurate Quantum Monte Carlo Calculations
Dario Alfè, University College London
Allocation: 1 Million Core-Hours

Multi-Scale Modeling of Catalytic Interfaces Based on 2D Sub-Nano Surface-Deposited Clusters
Anastassia N. Alexandrova, University of California, Los Angeles
Allocation: 1 Million Core-Hours

Port ACES III and SIAL
Erik Deumens, University of Florida
Allocation: 500,000 Core-Hours

Machine Learning for the Exploration of Chemical Compound Space
O. Anatole von Lilienfeld, Argonne National Laboratory
Allocation: 1 Million Core-Hours

Computer Science

Parallel Run-Time Systems
Jeff Hammond, Argonne National Laboratory
Allocation: 4 Million Core-Hours

Charm++ and Its Applications
Laxmikant V. Kale, University of Illinois at Urbana-Champaign
Allocation: 1.5 Million Core-Hours

Parallel Boost Graph Library
Andrew Lumsdaine, Indiana University
Allocation: 100,000 Core-Hours

SciDAC Scalable Data Management Analysis and Visualization
Michael E. Papka, Argonne National Laboratory
Allocation: 900,000 Core-Hours

Visualization and Analysis Research and Development for Argonne Leadership Computing Facility
Michael E. Papka, Argonne National Laboratory
Allocation: 500,000 Core-Hours

Distributed File Systems for Exascale Computing
Ioan Raicu, Illinois Institute of Technology
Allocation: 350,000 Core-Hours

I/O Forwarding Scalability Layer
Rob Ross, Argonne National Laboratory
Allocation: 1.5 Million Core-Hours

Parallel Performance Evaluation Using the TAU Performance System
Sameer Shende, ParaTools, Inc.
Allocation: 100,000 Core-Hours

TotalView Debugger on Blue Gene/P
Peter Thompson, TotalView Technologies
Allocation: 250,000 Core-Hours

Earth Science

Dynamic Downscaling of Climate Models
V. Rao Kotamarthi, Argonne National Laboratory
Allocation: 1.25 Million Core-Hours

Large Eddy Simulations of Atmospheric Convection
David Romps, Lawrence Berkeley National Laboratory
Allocation: 700,000 Core-Hours

Sensitivity and Uncertainty of Precipitation of the GFDL High-Resolution Model
Laura Zamboni, Argonne National Laboratory
Allocation: 100,000 Core-Hours

Energy Technologies

Molecular Modeling of Nanoscale Transport Pertinent to Energy Conversion and Storage
Soumik Banerjee, Washington State University
Allocation: 250,000 Core-Hours

Oxygen-Sensitivity Problem of Hydrogenases
Martin Stiebritz, ETH Zurich
Allocation: 1 Million Core-Hours

Engineering

A Computational Study of a Proprietary Parallel, Arbitrary Cell Type Code Used by G.E. Global Research
Ramesh Balakrishnan, Argonne National Laboratory
Allocation: 1 Million Core-Hours

Porting ExaFMM to Blue Gene/P Architecture and Turbulence Validation Studies
Lorena A. Barba, Boston University
Allocation: 1 Million Core-Hours

Quantum Lattice Algorithm for Quantum Turbulence
George Vahala, College of William & Mary
Allocation: 300,000 Core-Hours

Fusion Energy

Global Gyrokinetic Particle-in-Cell Investigations of ITER-Relevant Fusion Plasmas
William M. Tang, Princeton University, PICSciE and Princeton Plasma Physics Laboratory
Allocation: 5 Million Core-Hours

Materials Science

Quantum Monte Carlo Methods for Solids and Liquids
Dario Alfè, University College London
Allocation: 500,000 Core-Hours

SPaSM Molecular Dynamics Simulations of Material Dynamics
Timothy C. Germann, Los Alamos National Laboratory
Allocation: 500,000 Core-Hours

First-Principle Investigations of Oxygen Defects in Metal-Oxide-Metal Heterostructures
Olle Heinonen, Argonne National Laboratory
Allocation: 500,000 Core-Hours

Modeling Oil Properties with Molecular Dynamics
Detlef Hohl, Shell International E&P, Inc.
Allocation: 150,000 Core-Hours

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

Wavelet Basis Set in Density Functional Theory Methods for Photoelectric Materials
Alvaro Vazquez-Mayagoitia, Argonne National Laboratory
Allocation: 900,000 Core-Hours

Nuclear Energy

Modeling of Defects in Materials for Energy Applications
John J. Low and Marius Stan, Argonne National Laboratory
Allocation: 500,000 Core-Hours

Physics

3D Simulations of Magnetorotational Core-Collapse Supernovae
Sean Couch, The University of Chicago
Allocation: 5 Million Core-Hours

NEK5000
Paul Fischer, Argonne National Laboratory
Allocation: 1 Million Core-Hours

Electromagnetics
Misun Min, Argonne National Laboratory
Allocation: 500,000 Core-Hours

First-Principles Calculation of Laser-Induced Ultrafast Magnetism
Guoping Zhang, Indiana State University
Allocation: 1.5 Million Core-Hours

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CONTACT

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