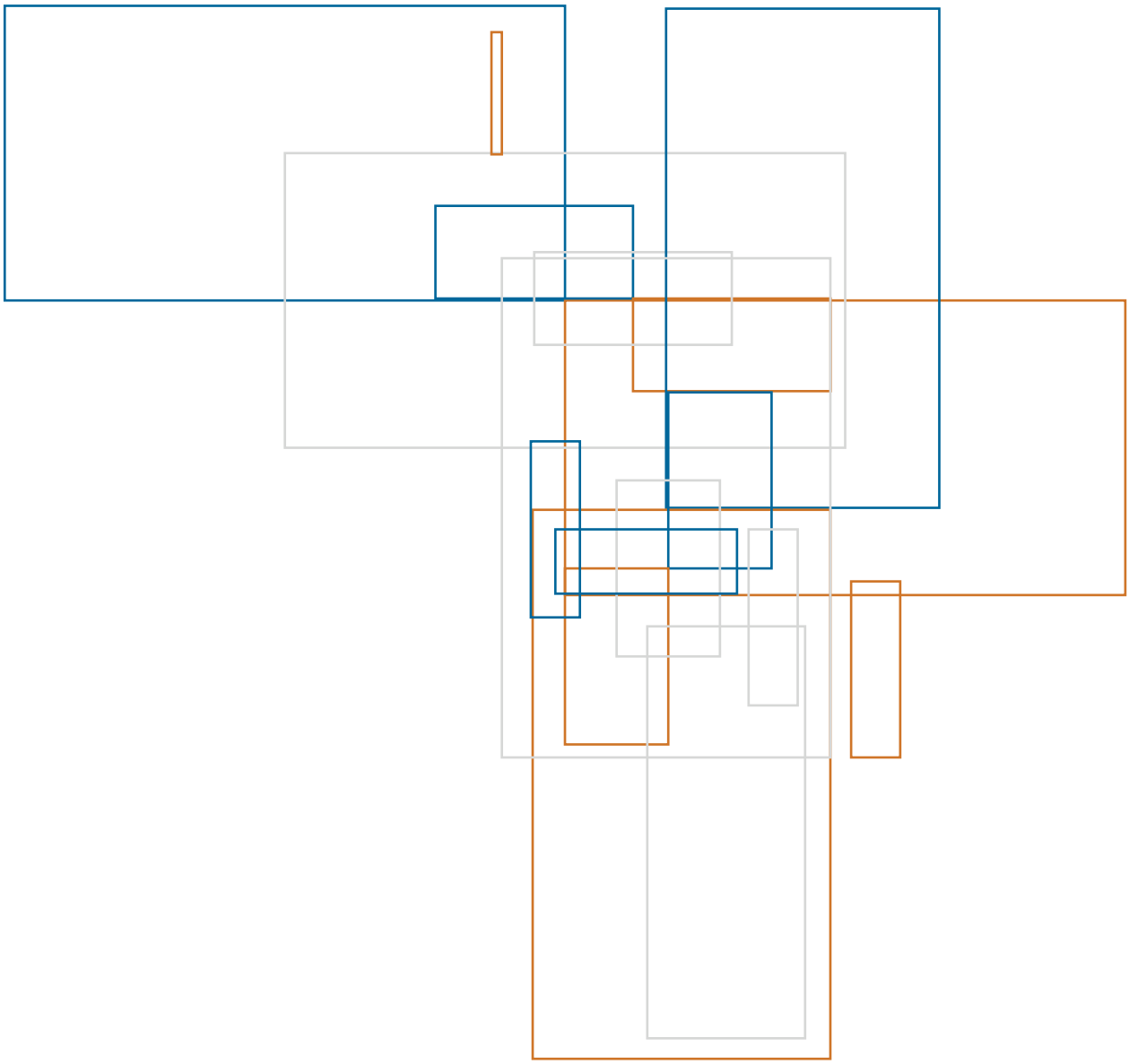

U.S. DEPARTMENT OF ENERGY

INCITE

LEADERSHIP COMPUTING

IN REVIEW

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

PRODUCTION TEAM

Team Leader: Julia C. White

Publication Director: Dawn Levy

Editors: Priscilla Henson, Dawn Levy

Contributing Science Writers: Cheryl Drugan, Eric Gedenk, Kathryn Jandeska, Scott Jones, Dawn Levy, Caitlin Rockett, Leo Williams, Laura Wolf

Graphic Designer: Jason Smith

Reviewers: Arthur Bland, Susan Coghlan, James J. Hack, Bronson Messer, Paul Messina, Michael Papka, Katherine Riley, Julia C. White

Advisors: Ashley Barker, Jayson Hines, David Martin

CONTACT
Julia C. White
INCITE Manager
Phone: 865-241-8796
whitejc@DOEleadershipcomputing.org

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Contents

INCITE Accelerates Research Breakthroughs with Leadership Computing

Since 2003 the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program has promoted transformational advances in science and technology through large allocations of computer time, supporting resources, and data storage. From modeling hurricanes that put people and property at risk to simulating combustion instabilities in power plant turbines and vehicle engines, INCITE projects aim to accelerate breakthroughs in fields in which major advancements would not be probable or even possible without supercomputing.

The INCITE program was created in 2003 by Raymond Orbach, then director of the Department of Energy's (DOE's) Office of Science, and managed by DOE Office of Science Advanced Scientific Computing Research (ASCR) staff until 2009. In a talk to the Council on Competitiveness Orbach remarked, "It is often said that science is based on two pillars, namely experiment and theory. In fact, high-end computation, especially through simulation, is the third pillar of science. It is actually a staple support as well. It gives us the ability to simulate things which cannot be done either experimentally or for which no theory exists—simulations of complex systems which are simply too hard or so far are not amenable to analytic approaches."

By today's standards INCITE started off modestly. In 2004 three projects received a total of nearly 5 million processor hours from Lawrence Berkeley National Laboratory's (LBNL's) National Energy Research Scientific Computing Center (NERSC). Since 2008 the program has been focused on utilizing DOE's Leadership Computing Facilities (LCFs),the primary source from which researchers can obtain the largest single-award time allocations anywhere on some of the world's most powerful computing systems, including a Cray XT5 called Jaguar with 224,256 processing cores yielding a peak performance of 2.33 thousand trillion calculations each second (2.33 petaflops) and an IBM Blue Gene/P called Intrepid with 163,840 processing cores yielding a peak performance of 557 trillion calculations per second. For the 2011 calendar year, 57 INCITE awardees received a total of 1.7 billion processor hours. The allocations averaged 27 million hours, with one project receiving more than 110 million hours. From INCITE's inception through the end of 2011, researchers from academia, government laboratories, and industry will have been allotted more than 4.5 billion processor hours to explore the natural world from subatomic particles to the vast cosmos, and the engineered world from cars and concrete to DNA sequencers and room-temperature superconductors.

The LCFs began joint management of INCITE in 2009 and made the first supercomputing allocations under such management in 2010. To commemorate the completion of the second year of the program's joint management by DOE's Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory (Argonne) and Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory (ORNL), we're taking the opportunity to present some of the scientific accomplishments of our users. This publication, which provides a comprehensive listing of INCITE projects in the appendix, highlights select projects. They include simulations to make personalized genomics quick and affordable; explore corrosion in building materials and carbon sequestration underground; optimize turbulent combustion in power and propulsion devices; and develop next-generation catalysts, computer chips, and nuclear reactors. Some elucidate biomass conversion for energy production and supercapacitors for energy storage. Others contribute to building a deeper understanding of phenomena from earthquakes to supernovas.

If mathematics is the language of science, computation is its workhorse—and will be for the foreseeable future. Unprecedented computing power allows scientists and engineers to approach grand challenges, from understanding the nature of dark matter or the molecular basis of disease to designing a car battery that can last for 500 miles, a biofuel that is economically viable, or a fusion reactor that can provide clean energy. Exploring the frontiers of science and technology and pushing farther and faster to reach breakthroughs requires enormous computing power to solve the equations behind the greatest enigmas of our time, such as grasping what is happening to our planet's climate and figuring out how to accelerate the arrival of sustainable energy technologies. The complexity of these problems leads to a voracious appetite for computing resources on the part of the scientific community. Through the INCITE program the world's most advanced computational researchers will continue to receive substantial allocations on some of the world's most powerful supercomputers.

To ensure INCITE scientists make the most of the supercomputers, the LCFs provide a staff of highly skilled high-performance computing (HPC) experts and computational scientists. These specialists are professionals in fields including chemistry, physics, astrophysics, mathematics, numerical analysis, and computer science, but they are also experts in designing code and optimizing it to run on LCF systems. Numerical experiments that incorporate high resolutions and employ realistic physical models are starting

to produce results researchers can confidently compare to experimental or theoretical ones, opening the door to a capability the scientific community has not had to this point: predictive simulation.

INCITE projects continue to attract high-caliber callouts. "At Oak Ridge National Laboratory," President Obama said in his 2011 State of the Union Address, "they're using supercomputers to get a lot more power out of our nuclear facilities." *They*, in this context, is the Consortium for Advanced Simulation of Light Water Reactors, an ORNL-based collaboration of national laboratories, universities, private industry, and other organizations. ORNL physicist Thomas Evans and colleagues use Denovo, an application that solves the Boltzmann equation describing the statistical distribution of individual particles in a fluid, to simulate radiation.

Whether it's gaining a better understanding of the universe or engineering solutions for a growing, energy-hungry populace, the investigations enabled by INCITE are making the world a smarter, more sustainable place. We are proud to tell the story of INCITE's role to date in advancing the frontiers of human knowledge for the benefit of all.

Still, huge challenges remain as researchers strive to make the discoveries that will revolutionize energy, transportation, construction, manufacturing, and more. To borrow from *The X-Files* television series of earlier years, the truth is out there. Supercomputers will help members of the scientific community discover it sooner. And INCITE will remain their premier means of accessing these unique resources.

James J. Hack
Director, National Center for Computational Sciences, which houses the OLCF

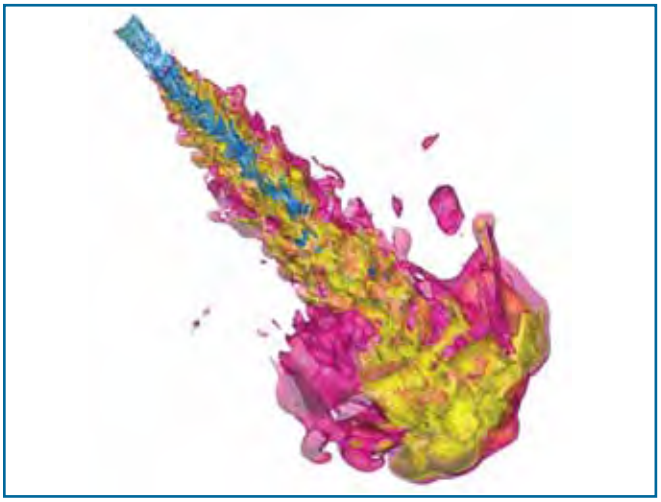
Michael E. Papka
Director, ALCF

Julia C. White
Program Manager, INCITE

Modeling Turbulent Combustion Speeds Design of Power and Propulsion Devices

ABSTRACT

Simulations of turbulent fuel combustion require powerful supercomputers and generate data used to predict—and optimize—performance of engines, turbines, and other devices for clean energy. One possible payoff is fuel efficiencies at least 25 percent higher in advanced engines employing compression ignition to burn lean fuels at relatively low temperatures.



High-fidelity LES of direct-injection processes in internal-combustion engines provides an essential component for development of high-efficiency, low-emissions vehicles. Here LES reveals how fuel from a state-of-the-art injector mixes with air inside an engine cylinder. Image courtesy Joseph Oefelein and Daniel Strong, Sandia

Air and fuel mix violently during turbulent combustion. The ferocious mixing needed to ignite fuel and sustain its burning is governed by the same fluid dynamics equations that depict smoke swirling lazily from a chimney. Large swirls spin off smaller swirls and so on. The multiple scales of swirls pose a challenge to the supercomputers that solve those equations to simulate turbulent combustion. Researchers rely on these simulations to develop clean-energy technologies for power and propulsion.

A team led by mechanical engineers Joseph Oefelein and Jacqueline Chen of Sandia National Laboratories (Sandia) simulates turbulent combustion at different scales. A burning flame can manifest chemical properties on small scales from billionths of a meter up to thousandths of a meter, whereas the motion of an engine valve can exert effects at large scales from hundredths of a meter down to millionths of a meter. This multiscale complexity is common across all combustion applications—internal combustion engines, rockets, turbines for airplanes and power plants, and industrial boilers and furnaces.

Chen and Oefelein were allocated 113 million hours on the OLCF's Jaguar supercomputer in 2008, 2009, and 2010 to simulate autoignition and injection processes with alternative fuels. For 2011 they received 60 million processor hours for high-fidelity simulations of combustion in advanced engines. Their team uses simulations to develop predictive models validated against benchmark experiments. These models are then used in engineering-grade simulations, which run on desktops and clusters to optimize designs of combustion devices using diverse fuels. Because industrial researchers must conduct thousands of calculations around a single parameter to optimize a part design, calculations need to be inexpensive.

"Supercomputers are used for expensive benchmark calculations that are important to the research community," Oefelein said. "We [researchers at national labs] use the Oak Ridge Leadership Computing Facility to do calculations that industry and academia don't have the time or resources to do."

The goal is a shorter, cheaper design cycle for U.S. industry. The work addresses DOE mission objectives to maintain a vibrant science and engineering effort as a cornerstone of American economic prosperity and lead the research, development, demonstration, and deployment of technologies to improve energy security and efficiency. The research, which supports a 20-year DOE priority to expand the frontiers of scientific discovery through leadership-class computing, was featured in *Breakthroughs 2008*, a report about major advances in computational science.

Making combustion more efficient would have major consequences given our reliance on natural gas and oil. Americans use two-thirds of their petroleum for transportation and one-third for heating buildings and generating electricity. "If low-temperature compression ignition concepts employing dilute fuel mixtures at high pressure are widely adopted in next-generation autos, fuel efficiency could increase by as much as 25 to 50 percent," Chen said.

Complementary codes

Chen uses a direct numerical simulation (DNS) code called S3D to simulate the finest microscales of turbulent combustion on a three-dimensional (3D) virtual grid. The code models combustion unhindered by the shape of a device. These canonical cases emulate physics important in both fast ignition events and slower eddy turbulence and provide insight into how flames stabilize, extinguish, and reignite.

Oefelein, on the other hand, uses a large eddy simulation (LES) code called RAPTOR to model processes in laboratory-scale

burners and engines. LES captures large-scale mixing and combustion processes dominated by geometric features, such as the centimeter scale on which an engine valve opening might perturb air and fuel as they are sucked into a cylinder, compressed, mixed, burned to generate power, and pushed out as exhaust.

Whereas DNS depicts the fine-grained detail, LES starts at large scales and works its way down. The combination of LES and DNS running on petascale computers can provide a nearly complete picture of combustion processes in engines.

> We [researchers at national labs] use the Oak Ridge Leadership Computing Facility to do calculations that industry and academia don't have the time or resources to do.—Joseph Oefelein, Sandia National Laboratories

"Overlap between DNS and LES means we'll be able to come up with truly predictive simulation techniques," Oefelein said. Today experimentalists burn fuel, collect data about the flame, and provide the experimental conditions to computational scientists, who plug the equations into a supercomputer that simulates a flame with the same characteristics as the observed flame. Researchers compare simulation to observation to improve their models. The goal is to gain confidence that simulations will predict what happens in the experiments. New products could then be designed with inexpensive simulations and fewer prototypes.

In a high-fidelity DNS with cells just 5 millionths of a meter wide, Chen's team modeled combustion in a canonical high-pressure, low-temperature domain to investigate processes relevant to homogeneous charge compression ignition. Another simulation, using 7 billion grid points, explored syngas, a mix of carbon monoxide and hydrogen that burns more cleanly than coal and other carbonaceous fuels. It used 120,000 (approximately half) of Jaguar's processors and generated three-quarters of a petabyte of data.

Since their 2008 simulation of a hydrogen flame—the first to fully resolve detailed chemical interactions such as species composition and temperature in a turbulent flow environment—they have simulated fuels of increasing complexity. Because real-world fuels are mixtures, simulations use surrogates to represent an important fuel component. Current simulations focus on dimethyl ether (an oxygenated fuel) and n-heptane (a diesel surrogate). Simulations are planned for ethanol and iso-octane (surrogates for biofuel and gasoline, respectively).

Oefelein uses RAPTOR to investigate turbulent reacting flows in engines. In a GM-funded experimental engine designed at the University of Michigan and used by the research community as a benchmark, he explores phenomena such as cycle-to-cycle variations, which can cause megaknock—an extreme form of the "bouncing marbles" sound sometimes heard in older engines. The fuel injection, air delivery, and exhaust systems are interconnected, and pressure oscillations have huge effects on engine performance. "Megaknock can do significant damage to an engine in one shot," said Oefelein. He noted that combustion instabilities also plague power plants, where fear forces designers of gas turbines to make conservative choices that lessen performance. "Combustion instabilities can destroy a multimillion dollar system in milliseconds," Oefelein said.

Petascale simulations will light the way for clean-energy devices and fuel blends that lessen combustion instabilities. The data they generate will inform and accelerate next-generation technologies that increase energy security, create green jobs, and strengthen the economy.

Contributors/Authors

Jacqueline Chen, Joe Oefelein, Gaurav Bansal, Hemanth Kolla, Bing Hu, Guilhem Lacaze, and Rainer Dahms, Sandia; Evatt Hawkes, University of New South Wales; Ray Grout, National Renewable Energy Laboratory; Andrea Gruber, SINTEF (the Foundation for Scientific and Industrial Research at the Norwegian Institute of Technology)

Principal Collaborators

The contributors work with Ramanan Sankaran of ORNL for computational science and Hongfeng Yu and Ajith Mascarenhas of Sandia for visualization and topology feature tracking.

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Publications

J. Chen. 2011. Plenary Paper "Petascale Direct Numerical Simulation of Turbulent Combustion—Fundamental Insights Towards Predictive Models," *Proceedings of the Combustion Institute* 33: 99–123.

C. Yoo, R. Sankaran, and J. Chen. 2010. "3D Direct Numerical Simulation of a Turbulent Lifted Hydrogen/Air Jet Flame in Heated Coflow: Stabilization and Structure." *Journal of Fluid Mechanics* 460: 453–481.

J. Frank, S. Kaiser, and J. Oefelein. 2010. "Analysis of Scalar Mixing Dynamics in LES Using High-Resolution Imaging of Laser Rayleigh Scattering in Turbulent Non-Reacting Jets and Non-Premixed Jet Flames." *Proceedings of the Combustion Institute* 33: 1373–1381.

B. Hu, M. Musculus, and J. Oefelein. 2010. "Large Eddy Simulation of a Transient Gas Jet with Emphasis on Entrainment during Deceleration." *SAE World Congress*, Paper 2010-01-1133, April 13–15. Detroit, MI.

Advanced Computing Aids Design of Next-Generation Nuclear Reactors

ABSTRACT

The United States is committed to developing new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global demand. Advanced simulation and modeling are key components in this strategy.

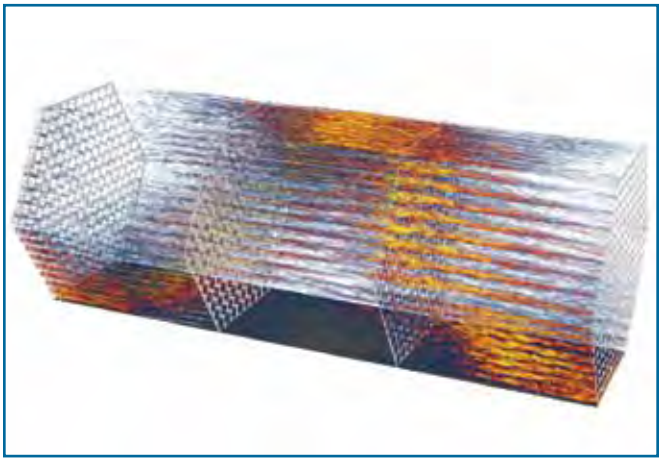
Advanced computing can help designers improve the safety and reliability of the next generation of nuclear reactors, providing a virtually carbon-free energy option and leading the world in industrial innovations.

As part of the work toward this goal, the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing simulation capabilities to leverage U.S. LCFs to address all aspects of the nuclear fuel cycle. In particular NEAMS seeks to enable engineers to probe the fundamental processes central to nuclear power generation in detail.

Nuclear reactors are typically very sparsely instrumented, and detailed information from inside them is generally not available. Historically, limited computing resources have constrained simulations used to develop reactor designs to basic one-dimensional models with model parameters empirically determined from simplified, benchtop experiments. "Advanced simulation is viewed as critical in bringing new reactor technology to fruition in an economical and timely manner," said Argonne senior computational scientist Paul Fischer.

Fischer is part of Argonne's Simulation-Based High-Efficiency Advanced Reactor Prototyping (SHARP) group responsible for the reactor performance code, which is a NEAMS program element. The SHARP group focuses on simulating detailed spatial distributions and dynamic behavior of two key physical phenomena in the reactor: the neutron transport and fission processes that generate heat and the thermal hydraulics—the coolant flow that transports heat out of the reactor core to the steam turbines that generate electricity. "From a computational modeling standpoint, a reactor represents a massively complex and interrelated set of physical phenomena," said Fischer.

The highly turbulent flows and complex geometries in a reactor present particular challenges for thermal hydraulics modeling. The SHARP approach is based on a hierarchy of simulation tools ranging from DNS of turbulence, performed in conjunction with University of Illinois–Urbana-Champaign doctoral student Reetesh Ranjan and his advisor, Carlos Pantano, to coarser models based on LES, Reynolds-averaged Navier-Stokes (RANS), and lumped-parameter models. Each level of coarsening represents a performance gain, but at the cost of model fidelity. The more expensive DNSs and LESs are backed up by experimental comparison, when data are available. The simulations can in turn be used to validate the faster RANS and lumped-parameter models, which can rapidly explore parameter space in a design scenario.



Shown is the velocity distribution in a 217-pin nuclear reactor subassembly computed on the ALCF's IBM Blue Gene/P supercomputer, Intrepid. Image courtesy Paul Fischer, Argonne, and Hank Childs, LBNL

"In the past there were only two levels to the hierarchy—experiment and lumped models," noted Fischer. "With high-performance computing we have the ability to explore any point in the parameter space in detail using first principles."

Thermal striping and coolant mixing

Two issues are the primary focus of the SHARP thermal hydraulics analysis: thermal striping—temperature fluctuations generated when two (or more) streams of coolant at different temperatures combine into a single stream—and coolant mixing in fuel subassemblies.

The team uses the Nek5000 computational fluid dynamics (CFD) code developed by Fischer and colleagues to conduct large-scale DNSs and LESs of turbulent thermal transport. The detailed simulations are performed using time awarded through the INCITE program on the ALCF's IBM Blue Gene/P, Intrepid, which is one of the fastest computers in the world.

Thermal striping is of great interest to nuclear engineers because temperature fluctuations can cause metal fatigue and ultimately lead to component failure. Recent Nek5000 analysis of thermal striping on Intrepid identified a fundamental process that can strongly influence thermal fluctuations in a reactor outlet plenum (or reservoir). As part of its code validation plan, Argonne has built an experimental mock-up of a plenum that can support either flush-mounted or protruding jet inlets.

The Nek5000 simulations demonstrated that the flush-mounted configuration leads to unstable jets and enhanced thermal striping. The addition of a few centimeters of material to form protruding inlets prevents secondary flows from interfering with the jets, leading to a stable configuration. The unstable configuration could not be captured with RANS simulations.

"This is an example of where having high-performance computing and a variety of simulation tools really pays dividends," said Fischer. The Argonne plenum experiment has just come online, and the SHARP team is eagerly awaiting the opportunity to make detailed comparisons with the data.

Advanced simulation is viewed as critical in bringing new reactor technology to fruition in an economical and timely manner.—Paul Fischer, Argonne National Laboratory

Validation is an important component of the SHARP project. Last year the Organisation for Economic Co-operation and Development/Nuclear Energy Agency conducted a blind benchmark test to study thermal striping in a T-junction, in which cold flow in a pipe is mixed with hot flow from an adjoining one.

Participants were provided with experimental data in two inlet branches and asked to predict the results in the outlet branch. The Nek5000 submission, using 21 million gridpoints and 1 day of simulation time on 16,384 cores of Intrepid, was ranked first in temperature prediction and sixth in velocity prediction of 29 entries from around the world. The computational mesh was prepared using other tools and then fed to Nek5000 through the framework central to the overall SHARP project. The team has been performing additional simulations on Intrepid to explore important parameters that are not readily accessible through experiments.

Mixing of coolant in reactor subassemblies is another area in which HPC is proving its value. Nek5000 has been used to simulate the details of the turbulent mixing process within reactor pin bundles. These computations are some of the largest performed to date with Nek5000 and involve more than a billion gridpoints on unstructured meshes. These first-ever LESs of wire-wrapped fuel pins at design-level pin counts used 65,000 cores of Intrepid in a series of 60-hour runs over several weekends in a row for a total of 20 million CPU hours. Intrepid ran flawlessly, without interruption or downtime, for each of the runs. The Nek5000 results have been used to validate RANS models that in turn have been used to explore a variety of mixer designs in the fuel assemblies. The simulations are enabling researchers to gain an understanding of the fundamental thermal mixing phenomena within reactor subassemblies—in particular focusing on understanding the mechanisms that cause existing models to greatly underpredict the mixing observed in simple experiments.

"The NEAMS work is really a team effort," said Fischer. "It engages mathematicians, computer scientists, physicists, and nuclear engineers in developing advanced modeling capabilities—algorithms, software, verified code, and validated use cases—which can lead to improved safety and economy of new designs."

Contributors/Authors

Paul Fischer, Elia Merzari, Aleksandr Obabko, and W. David Pointer, Argonne

Principal Collaborators

Hank Childs of LBNL provides visualization support for the team.

Funding

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Publications

E. Merzari et al. 2010. "Numerical Simulation of the Flow in Wire-Wrapped Pin Bundles: Effect of Pin-Wire Contact Modeling." *Proceedings of the Computational Fluid Dynamics for Nuclear Reactor Safety Applications (CFD4NRS-3) Workshop*, Bethesda, MD, September 14–16.

E. Merzari, W.D. Pointer, and P. Fischer. 2010. "Proper Orthogonal Decomposition of the Flow in a T-Junction." *Proceedings of the 2010 International Congress on Advances in Nuclear Power Plants (ICAPP 2010)*, paper 10335, San Diego, CA, June 13–17.

E. Merzari et al. 2010. "On the Numerical Simulation of Thermal Striping in the Upper Plenum of a Fast Reactor." *Proceedings of the 2010 International Congress on Advances in Nuclear Power Plants (ICAPP 2010)*, paper 10334, San Diego, CA, June 13–17.

R. Ranjan, C. Pantano, and P. Fischer. 2010. "Direct Simulation of Turbulent Swept Flow Over a Wire in a Channel." *Journal of Fluid Mechanics* 651: 165–209.

Breakthrough Fusion Simulations Shed Light on Plasma Confinement

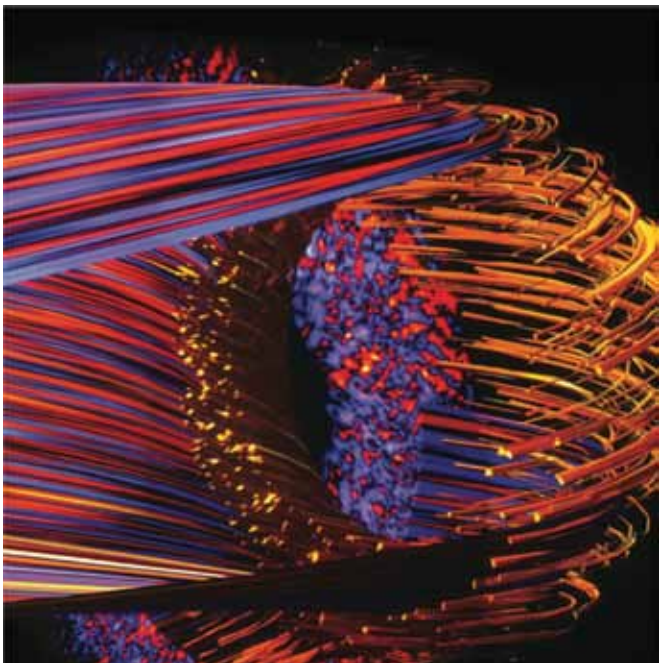
ABSTRACT

Researchers are using Oak Ridge and Argonne leadership-class computing resources to push fusion computer codes and associated algorithms closer to defining plasma confinement properties required to ignite the ITER experimental fusion reactor. The achievement is an important step toward developing a commercially viable, clean, limitless energy source.

A research team led by William Tang of DOE's Princeton Plasma Physics Laboratory (PPPL) is developing a clearer picture of plasma confinement properties in an experimental device that will pave the way to future commercial fusion power plants. Tang, who is also a professor at Princeton University, focuses on advanced simulation capabilities relevant to ITER, a multibillion-dollar international experimental device being built in France and involving the partnership of seven governments representing more than half of the world's population. If ITER is capable of sustaining effective fusion reactions, in which the fusion energy produced exceeds the input energy by more than an order of magnitude, humanity may well be on its way to a clean, safe, and limitless source of energy. Over the past 3 years using the ALCF's and OLCF's resources, Tang's team has made continual improvements to tools essential for computationally solving fusion problems.

Fusion of light nuclides (e.g., deuterium and tritium) forms the bulk of steady energy release in the universe. To build the scientific foundations needed to develop fusion as a sustainable energy supply, a key component is the timely development of an integrated high-fidelity simulation with experimentally validated predictive capability for magnetically confined fusion plasmas. Using magnetic fields is the most efficient approach to confining a plasma under conditions necessary to sustain a fusion reaction. An associated challenge is understanding, predicting, and controlling instabilities caused by microturbulence in such systems. By significantly increasing the transport rate of heat, particles, and momentum across the confining magnetic field in a tokamak such as ITER, microturbulence can severely limit the energy confinement time and therefore a machine's performance and economic viability. Understanding and possibly controlling the balance between these energy losses and the self-heating rates of the fusion reaction are essential to ensuring the practicality of future fusion power plants.

"Since you're never going to get rid of all the thermodynamic 'free energy' in a hot, magnetically confined plasma," Tang said, "the losses generated by the persistent presence of plasma microtubulence feeding off of this free energy will ultimately determine the size and cost of a fusion reactor."



A global particle-in-cell simulation uses Weixing Wang's GTS code to show core turbulence in a tokamak. Image courtesy Scott Klasky, ORNL

Tang and his colleagues are working to understand how to control and mitigate such microturbulence to help ensure an economically feasible fusion energy system. Their investigations focus on two codes, GTC-P and GTS, which are both global particle-in-cell kinetic codes modeling the motion of representative charged particles and the interactions of those particles with the surrounding electromagnetic field.

This research aligns with the 20-year DOE priority to support ITER for developing fusion energy. The associated effort requires development of codes that can scale to huge numbers of processors and thereby enable efficient use of the most powerful supercomputers on the planet. Tang's INCITE experience working with some of the world's most powerful supercomputers is likely to serve him well in his new role as the U.S. principal investigator for a new international G8 Exascale Project in fusion energy. This HPC collaboration involves the United States (Princeton University with hardware access at Argonne), European Union (United Kingdom, France, and Germany with hardware access at the Jülich Supercomputing Centre), Japan, and Russia. It will explore the viable deployment of application codes as platforms move toward the exascale (supercomputers capable of a million trillion calculations per second).

Scaling to new heights

Enabled by the INCITE program, the leadership-class computing allocations to Tang, Stephane Ethier, Weixing Wang, and other colleagues—8 million processor hours on the OLCF's Jaguar supercomputer and 2 million on the ALCF's Intrepid supercomputer in 2008, 30 million hours at the OLCF and 6 million at the ALCF in 2009, and more than 45 million at the OLCF and 12 million at the ALCF in 2010—have allowed the team to improve its algorithms. Its scaling efforts helped the researchers make the most of HPC systems and culminated by demonstrating that the GTC-P code efficiently scaled up to use the full 131,072 cores of Intrepid.

> Since every simulation is inherently imperfect, you will want to continue to increase the physics fidelity of any advanced code, be it in physics, chemistry, climate modeling, biology, or any other application domain. So you will always have—and Mother Nature demands that you will always have—a voracious appetite for more and more powerful computational capabilities.—William Tang, Princeton Plasma Physics Laboratory and Princeton University

Overall this research has produced HPC capabilities for capturing insights into microturbulence, moving researchers closer to answering the key question of how turbulent transport and associated confinement characteristics differ in present-generation laboratory plasmas versus ITER-scale burning plasmas, which are at least three times larger. Continuing to successfully develop their codes, the researchers incorporated radial domain decomposition capability in a project led by coinvestigator Mark Adams of Columbia University. Results from this effort led to unprecedented efficiency for scaling turbulent transport from relatively small present-generation experiments (in which confinement is observed to degrade with increasing reactor size) to large ITER-scale plasmas. This capability is in turn enabling scientists to gain new insights into the physics behind the expected favorable trend whereby the plasma confinement will cease to degrade as plasma size increases.

Tang commented that the impressive capability of LCF machines is related to Moore's Law, an empirical observation that computing power doubles every 18 months and is projected to do so until 2015 or so. "Since every simulation is inherently imperfect, you will want to continue to increase the physics fidelity of any advanced code, be it in physics, chemistry, climate modeling, biology, or any other application domain. So you will always have—and Mother Nature demands that you will always have—a voracious appetite for more and more powerful computational capabilities," Tang said. "You have to come up with more and more creative algorithms that allow you to tap the compute power of the increasingly complex modern systems."

If the team can continue to successfully make use of such systems, the resulting large-scale simulations will create large amounts of data that will clog the flow of information into and out of processing cores, Tang pointed out. Accordingly, his team includes ORNL computational scientist Scott Klasky, the lead developer of the Adaptive Input/Output System, or ADIOS. This middleware expedites the movement of data into and out of the computer and to the I/O system. The contribution means HPC systems spend more time computing scientific answers and less time transferring data.

As ITER moves to the operational phase, the ability to use leadership computing resources to promptly harvest physics insights from such applications will be essential in guiding the experimental campaign.

Contributors/Authors

William Tang, PPPL and Princeton University

Principal Collaborators

Tang's team includes Mark Adams, Columbia University; Bruce Scott, Max-Planck Institut für Plasmaphysik; Scott Klasky, ORNL; and Stephane Ethier and Weixing Wang, PPPL.

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Publications

W. Wang et al. 2010. "Nonlinear Flow Generation by Electrostatic Turbulence in Tokamaks." *Physics of Plasmas* 17, no. 7: 072511.

K. Madduri et al. 2009. "Memory-Efficient Optimization of Gyrokinetic Particle-to-Grid Interpolation for Multicore Processors." Presented at SC09, Seattle, WA, March 2009.

W. Tang. 2008. "Scientific and Computational Challenges of the Fusion Simulation Project." SciDAC 2008 Conference Proceedings in *Journal of Physics: Conference Series* 125, no. 1: 012047.

S. Ethier et al.2008. "Large-Scale Gyrokinetic Particle Simulation of Microturbulence in Magnetically Confined Plasmas." *IBM Journal of Research and Development* 52: 105.

Chemistry and Materials Computations Speed Clean Energy Production and Storage

ABSTRACT

Researchers seek to understand, control, and design processes and products for clean energy, such as biomass conversion for energy production and supercapacitors for energy storage. With unprecedented speed, simulations are solving the electronic structures of industrially important catalysts and device interfaces to accelerate breakthroughs in chemistry, nanotechnology, and materials science.

Enterprises from energy production to environmental cleanup depend on chemistry. Catalysts, which make chemical reactions more likely, contribute to nearly 20 percent of all industrial products. In the United States three industries relying on catalysts—petroleum, chemicals, and pharmaceuticals—account for $1 trillion of the gross national product.

Catalysts are just one area of investigation for a multi-institutional team whose 70 publications in 3 years detail prodigious scientific output from the world's fastest chemistry simulations. Its work integrates experiment, theory, and simulation to explore a continuum from chemistry to materials science. The researchers aim to understand, control, and design technologies needed for clean energy. These efforts closely align with DOE's missions and its 20-year priority to support nanoscale science for new materials and processes.

"Our long-term goal is enabling the design of new generations of clean and sustainable technologies to produce, transmit, and store energy," said team leader Robert Harrison, a computational chemist at ORNL and the University of Tennessee who directs the Joint Institute for Computational Sciences, a partnership between the two organizations. "Key elements are a fundamental understanding of chemical and electronic processes at the atomic scale and ultimately effectively transferring this knowledge in partnership with experiment into the hands of people and industries interested in the next steps of R&D."

Through the INCITE program the researchers have been awarded more than 100 million processor hours since 2008. At the OLCF they calculate the electronic structures of large molecules and surfaces using scientific application codes called NWChem and MADNESS. The findings inform the development of processes, such as biomass conversion and fuel combustion, and products, such as batteries, fuel cells, and capacitors.

The electronic structure allows scientists to determine the positions and binding energies of atoms within molecules and responses to perturbations. Petascale computers speed complex calculations of molecular dynamics (MD) and quantum mechanics as substances undergo chemical transformation.

Chemistry and materials science simulations made possible through Robert Harrison's INCITE project have generated 70 scientific publications since 2008, many of which graced the covers of prestigious journals and dealt with topics from production of hydrogen for clean energy to development of graphene nanoribbons for power delivery. Collage courtesy Robert Harrison and Jason Smith, ORNL

"Some of the largest calculations are only feasible on the leadership computers, not just because of speedy processors, but because of other architectural features—the amount of memory, the amount and speed of the disks, the speed and other characteristics of the interprocessor communication," Harrison said.

A scientific paper by team member Edoardo Apra of ORNL was a 2009 Gordon Bell finalist after he and coauthors reported scaling NWChem to use most of Jaguar, ORNL's Cray XT5 supercomputer, to calculate the electronic structure of water clusters, which is important in chemistry at interfaces and in nucleation in the atmosphere. Because NWChem is a flagship application used throughout the community, getting it to run at petascale would have high impact. That was a special challenge, though, because the code employs distributed, shared memory instead of the message passing used by most codes. As a result of the team's efforts, though, NWChem has now joined four other scientific applications sustaining more than a petaflop on Jaguar.

Further feats of computational science

Chemistry and materials science are critical for innovation. ORNL theorist Bobby Sumpter, with lab colleagues Vincent

Meunier and Jingsong Huang, ran calculations of hundreds of teraflops on Jaguar to investigate a next-generation capacitor, a device that stores energy through charge separation at an electric double layer formed within porous materials. As transportation systems are electrified, fast charging of vehicles with such devices will be necessary. Iterating between simulation and experiment to reduce intermediate models, within 2 years Sumpter's team and collaborators at Rice University arrived at a practical device for high-power energy delivery. Their supercapacitor stores—and quickly discharges—a thousand times more energy than a conventional capacitor. Several challenges remain to be overcome, however, before a commercial device can be developed and deployed.

Some of the largest calculations are only feasible on the leadership computers, not just because of speedy processors, but because of other architectural features—the amount of memory, the amount and speed of the disks, the speed and other characteristics of the interprocessor communication. —Robert Harrison, Oak Ridge National Laboratory

"Because there's very little chemical or material change, supercapacitors can be cycled millions of times without significant degradation. In contrast, in a battery you're physically moving considerable matter around and inducing chemical change, so it's much harder to cycle more than a few thousand times," Harrison said. "We're familiar with the batteries in our laptops and cell phones dying after a year or two."

While capacitors don't seem chemically active, in fact a lot of chemistry is going on that's relevant to energy storage. Indeed, Sumpter and collaborators achieved high energy densities in supercapacitors by coupling chemistry with nanomaterials—specifically, graphene nanoribbons structured at the billionth-of-a-meter scale of atoms. They considered the smallest unit of structure needed to achieve an energy-storage function and modeled a supercapacitor as a carbon pore. An ion and the shell of solvent surrounding it can move into the pore. But in materials with pores too small for the entire solvation shell to enter, some solvent gets stripped off. The ions align into a nanowire structure as they pack into the pore. The pore size and the ion's tiny diameter determine the high capacitance.

Whereas Sumpter and collaborators simulate energy storage, other members of Harrison's team address energy production. "When growing corn for conversion into ethanol, a lot of lignin and cellulosic material is left over," Harrison said. "We could get energy out of it, and we could turn it into other useful chemicals—if only we had controllable, efficient processes."

To improve those processes, computational chemist Ariana Beste and experimental chemist A.C. Buchanan, both of ORNL, explore thermochemical degradation of plant materials. They study how molecular structures influence networks of chemical reactions. The rate of a reaction depends on the height of the energy barriers along paths between reactants and products and the fraction of molecules with enough energy to hurdle those barriers. One chemical reaction may lead to half a dozen products. Favoring a path that results in a specific product may necessitate understanding a hundred reaction paths.

Petascale simulations can quickly calculate the proportion of molecules with the requisites for a specific reaction—a herculean statistical challenge. Calculating which bonds between atoms in a molecule have the lowest energies, for example, reveals the optimal shape for a molecule to assume. That knowledge can speed design of processes faster than do trial and error or expert insight.

"Chemistry and materials sciences are sciences about the real world, which is complicated and messy, hard to characterize and control," Harrison said. "We're never going to be in a position to say we can replace chemistry with simulation. What we can say, confidently now, is that in increasingly large areas of our discipline, simulation and theory are equal and valued partners with experiment. Petascale computing is critical to accelerating scientific advancements."

Contributors/Authors

Robert Harrison and Bobby Sumpter, ORNL

Principal Collaborators

Principal scientific collaborators are Edoardo Apra, ORNL; David Dixon, University of Alabama; Karol Kowalski, Pacific Northwest National Laboratory (PNNL); and David Sherrill, Georgia Institute of Technology.

Funding

DOE Basic Energy Sciences and ASCR

Publications

G. Feng et al. 2010. "Ion Distribution in Electrified Micropores and Its Role in the Anomalous Enhancement of Capacitance." *ACS Nano* 4, no. 4 (April 5): 2382–2390.

W. Gordon et al. 2009. "Temperature Evolution of Structure and Bonding of Formic Acid and Formate on Reduced and Fully Oxidized CeO2(111)." *Physical Chemistry Chemical Physics* 11, no. 47: 11171–11183.

X. Jia et al. 2009. "Controlled Formation of Sharp Zigzag and Armchair Edges in Graphene Nanoribbons." *Science* 323, no. 5922 (March 27): 1701–1705.

J. Romo-Herrera et al. 2008. "An Atomistic Branching Mechanism for Carbon Nanotubes: Sulfur as the Triggering Agent." *Angewandte Chemie International Edition* 47, no. 16 (April 7): 2948–2953.

Jaguar Supercomputer Performs Most Advanced Earthquake Simulation

ABSTRACT

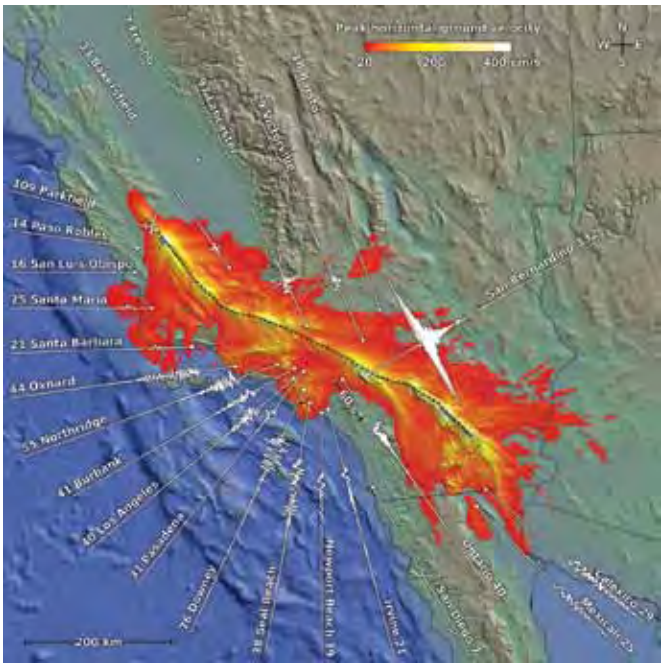
Simulations at the Oak Ridge Leadership Computing Facility help scientists develop and validate predictive models of earthquake processes and then use these models to better understand seismic hazard. Knowledge gained from the world's most advanced earthquake simulation, of a Southern California quake, should help building designers and emergency planners worldwide.

California straddles two major tectonic plates and is subject to relatively frequent, often major quakes. It should come as no surprise, then, that the most advanced simulation of an earthquake performed on a supercomputer focuses on California and its San Andreas Fault. A team led by Southern California Earthquake Center (SCEC) Director Thomas Jordan used ORNL's Jaguar supercomputer to simulate a magnitude-8 quake shaking a 125,000-square-mile area of Southern California and assess its regional impact. The simulation became one of six finalists for the 2010 Gordon Bell Prize, awarded to the world's most advanced scientific computing application, while providing insight valuable to seismologists, building designers, and emergency planners working to minimize the devastation of Southern California's inevitable next big shakeup.

"If you're studying earthquakes, Southern California is a good spot," said SCEC information technology architect Philip Maechling. "We've got a big plate boundary. The geology—a lot of it's in the desert—is well exposed. There's a lot of instrumentation in the region, ground motion sensors and GPS and strain meters. Plus there are a lot of people at risk. We're doing simulations in order to develop and validate predictive models of earthquake processes and then to use these models to better understand the seismic hazard in Southern California. The things we learn about earthquakes here should be applicable to earthquakes around the world."

Known as M8, the SCEC project simulates a 6-minute earthquake half again as powerful as the temblor that destroyed San Francisco in 1906—or 30 times as powerful as the quake that devastated Haiti in 2010. According to Maechling the center chose magnitude 8 because it is one of the largest quakes that could plausibly hit Southern California.

Maechling said the investigation on Jaguar was prompted by a change in philosophy by emergency management organizations after Hurricane Katrina. "Before Katrina they were asking, 'What's likely to happen? Give us the most probable scenarios that we're going to have to face.' But after Katrina they changed the question and said, 'Tell us, what's the worst that could happen?'" he noted. "My understanding is that they were changing the question because they want to be ready for not only the most likely but also the worst case."



Peak horizontal ground velocities derived from the M8 simulation reveal regions at risk during a magnitude-8 quake. Image courtesy Geoffrey Ely, University of Southern California

Unprecedented simulation

The San Andreas Fault forms the boundary between the Pacific and North American tectonic plates. The Pacific Plate includes a sliver of California and Baja California, as well as Hawaii and most of the Pacific Ocean, while the North American Plate includes the remainder of the United States, Greenland, and a hefty chunk of eastern Russia. The SCEC team simulated a 340-mile rupture on the San Andreas Fault and assessed the shaking it produces on a chunk of the earth's crust 500 miles long, 250 miles wide, and 50 miles deep. That chunk is home to 20 million people—about 1 in 15 Americans.

The M8 simulation meets a DOE 20-year priority to expand the frontiers of scientific discovery through advanced computation. It required Jaguar to address the size of the region (the simulation took 435 billion 40-cubic-meter cells) and the frequency of the seismic waves (the simulation calculated up to 2 hertz, or two cycles per second, without resorting to approximation).

No earthquake simulation of this scale has been able to directly calculate earthquake waves above 1 hertz. According to computational scientist Yifeng Cui of the San Diego Supercomputing Center (SDSC) at the University of California–San Diego (UCSD), each doubling in wave frequency requires

a 16-fold increase in computational resources. On the other hand, building engineers analyzing structural responses to strong ground motions use waves up to 10 hertz in their analyses, so M8 represents a milestone toward the larger goal of similar simulations at even higher frequencies.

"Going to these higher frequencies will allow us to capture a lot more parameters of the waves," noted San Diego State University (SDSU) geophysics professor Kim Olsen. "For example, you can characterize the waves by the displacement from side to side at a point, or the velocity of the point from side to side or up and down, or the acceleration of the point. With the low frequency we might be able to capture the displacement or even the velocities, but the acceleration of the point or the ground location is really a higher-frequency concept. We won't be able to capture that acceleration unless we go to higher frequencies—2 hertz or preferably even higher. And that acceleration is really needed for a lot of purposes, especially in structural engineering and building design."

> We're doing simulations in order to develop and validate predictive models of earthquake processes and then to use these models to better understand the seismic hazard in Southern California. The things we learn about earthquakes here should be applicable to earthquakes around the world.— Philip Maechling, Southern California Earthquake Center

The project's first simulation on Jaguar, in April 2010, ran for 24 hours and used nearly all of Jaguar's 223,000-plus processing cores. The simulation reached 220 trillion calculations per second, more than twice the speed of any previously completed large-scale seismic simulation. It used an earthquake wave propagation application program called AWP-ODC (for Anelastic Wave Propagation—Olsen-Day-Cui) based on a numerical method for calculating earthquake waves originally developed by Olsen. Solving a coupled system of partial differential equations defined on a staggered grid, the application calculates the rupture as it travels along the fault and the earthquake waves and resultant shaking as they spread through the region.

From 2009 to 2011, the ALCF and OLCF awarded Jordan's project a total of 42 million processor hours through the INCITE program. The researchers also received 2 million hours at the OLCF in 2010 through DOE's ASCR Leadership Computing Challenge, which awards supercomputing time to high-risk, high-impact projects.

M8 produced high-fidelity ground motions for all regions within the simulation because it used an accurate 3D model of Southern California's complex geology, which has been thoroughly analyzed after decades of oil exploration. Geology makes a profound difference in the way an earthquake plays out. Unfortunately, the sediment layers that fill valleys and underlie most populated areas shake longer and harder than other geologic forms. Sedimentary basins such as those below Los Angeles, San Fernando, and San Bernardino tend to trap earthquake waves, which then bounce back and forth rather than moving on. "Imagine a bathtub full of water," Olsen said. "If you kick the bathtub, the water will start sloshing back and forth in the tub. That's an analogy to what happens to seismic waves in a sedimentary basin."

The team compared results from the M8 simulation with data averaged from many real earthquakes. The average shaking seen in the simulation on rock sites (that is, areas other than sedimentary basins) matched very well with available data. The ground motion in sedimentary basins such as Los Angeles and Ventura was generally larger than predicted by the average data records, noted Olsen, but that discrepancy is readily explained by the fact that averaged records do not reflect effects caused by complex source propagation and 3D basin amplification in a specific earthquake. In particular, he noted, the simulation included long stretches in which the ground ruptured faster than the speed of a particular wave known as the shear wave. This supershear rupture created an effect analogous to a sonic boom and may account for the especially strong ground shaking in the basins. Additional M8 rupture scenarios planned within SCEC will explore this possibility.

Contributors/Authors

Thomas Jordan and Philip Maechling, USC

Principal Collaborators

Yifeng Cui, Kwangyoon Lee, and Jun Zhou of the SDSC at UCSD; Kim Olsen, Daniel Roten, and Steve Day of SDSU; Patrick Small and Geoffrey Ely of USC; Dhabaleswar Panda of Ohio State University–Columbus; and John Levesque of Cray Inc. make the simulations possible. Amit Chourasia of SDSC handles the visualizations.

Funding

NSF

Publications

Y. Cui et al. 2010. "Scalable Earthquake Simulation on Petascale Supercomputers." *Proceedings of the Supercomputing Conference, New Orleans, LA*, November. (Gordon Bell Prize finalist)

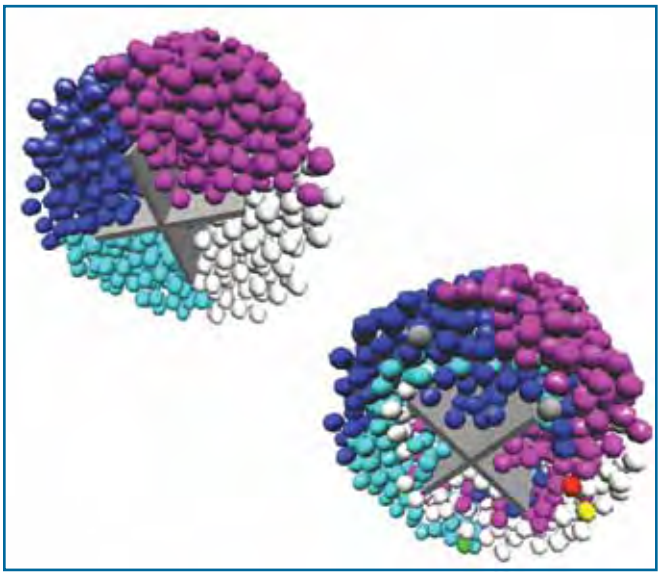
P. Chen et al. In press. "Rapid Full-Wave Centroid Moment Tensor (CMT) Inversion in a Three-Dimensional Earth Structure Model for Earthquakes in Southern California." *Geophysical Journal International*.

P. Chen, T. Jordan, and E. Lee. 2010. "Perturbation Kernels for Generalized Seismological Data Functionals (GSDF)." *Geophysical Journal International* 183, no. 2 (November): 869–883.

Leadership Computing Enables New Insights into the Flow Properties of Concrete

ABSTRACT

Flow simulations of thousands of particles on the Argonne Leadership Computing Facility's Blue Gene/P supercomputer are enabling new insights into how to measure and control flow properties of large-particle dense suspensions like concrete that cannot currently be accurately measured in industrial settings. A better understanding of these properties will help ensure the optimum performance of concrete and eliminate cost overruns.



Two frames of an animation show a preliminary test of the vane rheometer simulator using mono-sized spherical particles. Particles in each octant of the cylindrical system are color coded by their initial location. The top image shows the system at the start of the simulation. The bottom image shows the system after approximately two rotations of the vane blades. The bottom four octants have been cut away to show the rheometer vanes. Images and the software used to produce them were developed by Steven Satterfield, John Hagedorn, and John Kelso of NIST and Marc Olano of NIST and the University of Maryland–Baltimore County.

Concrete has been used for construction since ancient times. The word *concrete* is of Latin origin, indicating the likelihood that the ancient Romans were the first to use the substance. Many examples of Roman concrete construction remain in countries encircling the Mediterranean, where Roman builders had access to numerous natural cement deposits. Today concrete is the most widely used building material in the world, representing a $100 billion industry in the United States that is crucial for our nation's physical infrastructure. At least 7.5 cubic kilometers of concrete are made each year—more than 1 cubic meter for every person on Earth.

There is currently considerable interest in making concrete a more sustainable material by finding new ways to recycle it and changing its ingredients to reduce the amount of greenhouse gas generated during its production. (The manufacture of concrete's key ingredient, cement, accounts for about 5 to 8 percent of carbon dioxide worldwide.) However, changing ingredients (modifying the mix design) to use different materials may adversely affect concrete's flow characteristics. As new mix designs are developed to meet the world's needs while also being environmentally responsible, measuring and controlling concrete's rheological properties (the flow properties such as viscosity or resistance to flow) are key to satisfying performance specifications. Failure to control the flow of concrete on a job site—and the need to correct resulting errors—can lead to significant cost overruns and possibly performance sacrifices.

Researchers led by William George from the National Institute of Standards and Technology (NIST) are leveraging the computational resources of the Blue Gene/P high-performance computing system at the ALCF to shed light on the mechanisms that control the flow and spread of suspensions such as concrete. Insight from these studies has technological application in the building, coatings, water-treatment, food-processing, and pharmaceutical industries. Results from this work will also further DOE's mission to develop revolutionary new materials and processes.

Modeling the flow of concrete represents a great scientific and computational challenge. Concrete is a dense suspension composed of aggregates (such as sand and gravel) with sizes ranging over several orders of magnitude. A further complication is that the aggregates are embedded in a non-Newtonian fluid. *Non-Newtonian* means that the relationship between stress and shear rate is nonlinear and possibly strain-history dependent. Significant effects from aggregate shape and size variations exist that cannot be accounted for by modeling the aggregates as idealized spheres. As concrete undergoes shear flow, the shear-rate-dependent microstructures formed by the aggregates dynamically change as these microstructures are built up and destroyed over time.

Measuring the true rheological properties of fresh concrete is an unmet challenge. Laboratory devices that measure the way a suspension flows in response to applied forces—called rheometers—can only approximate rheological properties of suspensions because these devices gauge only torque and angular velocity. Without detailed knowledge of the flow in the rheometer, one cannot obtain fundamental rheological parameters such as viscosity and yield stress (resistance to initiating flow). Hence, computing the flow allows researchers to correctly interpret empirical measurements in terms of fundamental units.

"Analysis and visualization of the simulated flow enable us to develop a conceptual framework to understand important physical mechanisms that control the flow of such complex fluid systems," noted George.

Shedding light on key physical mechanisms

The Blue Gene/P supercomputer gives researchers the computing power to perfect their algorithms, test parameters such as system size and size distribution width of the suspended particles in a large-scale parallel approach, and gain a better understanding of dense suspension rheology.

There is no analytical solution for the stress and strain-rate fields based on the torque and angular velocity outputs of rheometers used for concrete. The investigators are seeking to apply large-scale parallel simulations to solve this problem of relating rheological properties such as viscosity as a function of shear rate to measured quantities such as torque and angular velocity.

"Realistic simulations of dense suspensions like concrete demand significant computational resources in order to produce results with predictive capability," said George. "To accurately simulate the flow of dense suspensions with sufficient detail with a representative range of suspended particle sizes and avoid any finite size effects, we must simulate systems with large numbers of particles and a correspondingly large volume of fluid. These simulations require the computational power of a machine such as the IBM Blue Gene/P Intrepid. Smaller compute resources lack the memory, compute power, and I/O speeds needed to complete these simulations."

Through their simulations the researchers have gained fundamental new insights into the yield stress of dense suspensions. Studies by the group indicate that particle contacts are an important factor in controlling the onset of flow in dense suspensions. Further, such interactions can be strongly influenced by the shape of the aggregates and lead to jamming effects that restrict the easy placement of concrete in forms. The researchers also discovered that for suspensions with a non-Newtonian fluid matrix, the local shear rates between aggregates strongly determine their rheological properties. These results have been validated against physical experiments with excellent agreement.

> Realistic simulations of dense suspensions like concrete demand significant computational resources in order to produce results with predictive capability.—William George, National Institute of Standards and Technology

Based on their previous studies of the flow of dense suspensions, the researchers found that representative models of concrete flowing in a vane rheometer (typically a cylindrical container that holds a sample of the fluid or suspension to be tested and a shaft with vanes extending from it) must include approximately 50,000 aggregates and 5 million fluid particles to obtain meaningful and predictive results. (Previous studies of dense suspensions in non-Newtonian fluids have used fewer than 1,000 aggregates.) This size simulation requires 16,000 to 32,000 processors on Intrepid to obtain results in a reasonable timeframe. Initial performance tests have shown that the simulator scales well on Intrepid in this processor range with this size system.

Results from this study will advance the understanding of the rheology of dense suspensions, enable the measurement science needed to better interpret rheometer output, and potentially lead to improved rheometer design. A successful outcome of this research will help solve critical outstanding problems in the cement and concrete industry in regards to quality control and assessment of fresh concrete properties as new source materials and novel mix designs are developed. Additionally, these results should transfer to a wide array of industries that use rheometers and mixers.

Contributors/Authors

William George and Nicos Martys, NIST

Principal Collaborators

Nicos Martys of NIST designs computer runs and conducts scientific data analysis. Edward Garboczi of NIST conducts scientific data analysis. Marc Olano of NIST designs and implements GPU-based visualization algorithms. Pascal Hébraud of Centre National de la Recherche Scientifique/École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris conducts scientific data analysis. Judith Terrill of NIST provides project management as well as data analysis and visualization. Additional support came from NIST collaborators Chiara F. Ferraris (experimental rheology, rheometer design consultation, and industry relations), John Hagedorn (analysis and visualization), Steve Satterfield (visualization), and John Kelso (infrastructure for visualization and analysis).

Funding

DOE Office of Science, ASCR, and Department of Commerce, NIST

Publications

N.S. Martys et al. 2010. "A Smoothed Particle Hydrodynamics-Based Fluid Model with a Spatially Dependent Viscosity: Application to Flow of a Suspension with a Non-Newtonian Fluid Matrix." *Rheologica Act* 49:1059–1069.

N.S. Martys et al. 2009. "Contact and Stress Anisotrophies in Start-Up Flow of Colloidal Suspensions." *Physical Review E* 80: 031401.

N.S. Martys et al. "Spatial-Temporal Correlations at the Onset of Flow in Concentrated Suspensions." Presented at the XV International Congress on Rheology, Monterey, CA, August 3–8, 2008.

N.S. Martys. 2005. "Study of a Dissapative Particle Dynamics-Based Approach for Modeling Suspensions." *Journal of Rheology* 49, no. 2: 401−424.

Elucidation of Stress Corrosion Cracking Mechanisms

ABSTRACT

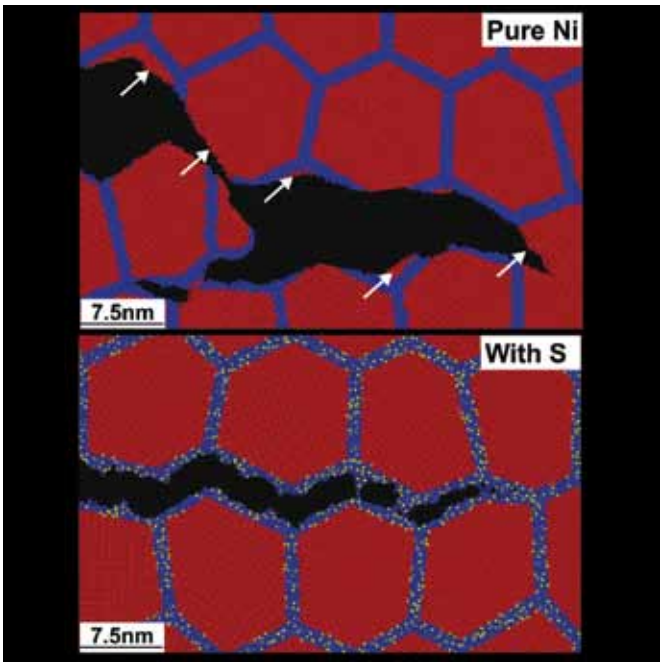
Petascale quantum mechanical-molecular dynamics simulations on Argonne's Blue Gene/P supercomputer encompass large spatiotemporal scales (multibillion atoms for nanoseconds and multimillion atoms for microseconds). They are improving our understanding of atomistic mechanisms of stress corrosion cracking of nickel-based alloys and silica glass—essential for advanced nuclear reactors and nuclear-waste management.

Stress corrosion—a concern in a wide range of sectors from municipal water supply systems to manufacturing, electricity, oil and gas transmission lines, high-temperature turbines, and transportation—is an enormously complex technological and economic problem, annually costing the United States about 3 percent of its gross domestic product. The performance and lifetime of materials used in nuclear and advanced power-generation technologies such as turbines, combustors, and fuel cells are often severely limited in corrosive environments or extreme high-pressure and high-temperature conditions in an environment that contains oxygen. Most critical is premature and catastrophic failure of materials resulting from chemically influenced corrosion. Safe and reliable operation is endangered by the uncertainties in stress corrosion cracking (SCC).

Investigating the environmental degradation of nickel-based alloys in advanced nuclear reactors and glass containers for nuclear waste is particularly key to DOE's aim to address the stress corrosion problem. Petascale simulations on the IBM Blue Gene/P supercomputer at the ALCF are providing a scientific team led by Priya Vashishta of USC with a crucial understanding of the atomistic mechanisms underlying SCC—the conditions influencing its initiation, dynamics, and growth.

"For the first time in the history of science and engineering, petascale computing and the emerging extreme computing will permit a simulation-based investigation of atomistic mechanisms in complex materials for energy technologies under extreme conditions of temperature, pressure, and radiation," Vashishta said.

The new knowledge may aid efforts to prevent SCC and predict the lifetime beyond which it may cause failure. The research addresses two of DOE's highest priorities for the Office of Science: mastering the ability to construct revolutionary new materials and processes atom by atom and exploring new forms of nuclear matter at high-energy densities and the extreme limits of stability.



Fracture simulations for nanocrystalline nickel without and with amorphous sulfide grain-boundary phases reveal a transition from ductile, transgranular tearing to brittle, intergranular cleavage. Image courtesy Hsiu-Pin Chen of USC et al., *Physical Review Letters* 104, 155502.

Current research in this area is building on the breakthrough success of earlier work conducted by the USC researchers. They performed the largest-ever (48 million atoms) chemically reactive MD simulation on 65,536 Blue Gene/P processors. "This milestone simulation answered a critical question for the design of next-generation nuclear reactors to address the global energy problem: how a minute amount of impurities segregated at grain boundaries of metal essentially alters its fracture behavior, resulting in catastrophic failure," stated Vashishta.

A prime example of such grain-boundary mechanochemistry is sulfur-segregation-induced embrittlement of nickel. The simulation revealed atomistic mechanisms of such embrittlement due to intergranular amorphization. Namely, sulfur impurity segregated to the boundaries between nickel crystalline grains causes the disordering of atomic arrangements at the grain boundaries, thereby weakening the material.

Simulation challenges

The research under way encompasses a rich and challenging set of applications involving simultaneous chemical, physical, and material processes that span length scales from interatomic distances to the mesoscale (lengths intermediate between atoms

and materials measured in microns). Chemically reactive domains evolve dynamically, and changes in configurations or charge distributions on surfaces and interfaces occur on timescales ranging from femtoseconds (quadrillionths of a second) to microseconds or longer. Simulations over such vast lengths and timescales require a continuous reevaluation of the domains over which the computational methods are applied, and straightforward communication across the quantum mechanical (QM) and MD boundary is vital. QM methods are essential to describing the chemistry, bond formation, and bond breaking between the metal and impurity atoms.

For the first time in the history of science and engineering, petascale computing and the emerging extreme computing will permit a simulation-based investigation of atomistic mechanisms in complex materials for energy technologies under extreme conditions of temperature, pressure, and radiation.—Priya Vashishta, University of Southern California

However, the straightforward, material-independent communication strategy between different computational methodologies required to solve material behavior in different regions of space remains elusive. To achieve a robust electronic and atomistic basis, the researchers found it is essential to develop first-principles models for all aspects of kinetics and dynamics, including the role of pH, charge distributions, temperature, pressure gradients, and electric field.

To address these computational challenges, researchers are employing their expertise in scalable algorithms, multimillion-to-billion-atom and microsecond MD simulations, and combined QM/MD simulations using the highest end of high-performance computing.

Hierarchical simulations of SCC contribute to making the problem tractable though challenging to implement on petaflops computing platforms such as the Blue Gene/P at Argonne. The researchers have integrated these methods into a single parallel framework by developing (1) optimal algorithms for varying degrees of length and timescales, (2) dynamic reordering of data and computation in simulation methods to achieve maximal spatial locality, and (3) communication of invariants and error tolerances across hierarchical levels.

Through these simulations, the scientists are investigating the fundamental mechanisms of SCC and nanoscale indentation of amorphous silica glass in the presence of water to atomistically understand the effect of water on damage. They are also exploring impurity segregation-induced embrittlement of nickel-aluminum alloys. Furthermore, they are studying chemical reactions on smooth and precracked samples under externally applied stresses in aqueous and gaseous environments.

The USC researchers have developed a reactive interatomic potential for MD simulations of silica-water systems and implemented a parallel reactive MD simulation program based on this interatomic potential on the Blue Gene/P system. To date they have performed validation simulations on water-silica systems and are currently simulating chemical reactions at silica crack surfaces and those at the silica surface due to cavitation bubble collapse. MD simulations of the damage to silica and ceramic coatings from nanobubble collapse in water under shock-wave compression are also being investigated.

Contributors/Authors

Priya Vashishta, USC

Principal Collaborators

The principal scientific collaborator is Aiichiro Nakano of USC, who will conduct petascale hierarchical QM/MD and accelerated MD simulations as well as collaborate on the authorship of any resulting publications.

Funding

DOE Office of Science, ASCR, and DOE NNSA

Publications

H. Chen et al. 2010. “Embrittlement of Metal by Solute Segregation-Induced Amorphization.” *Physical Review Letters* 104, no. 155502:1–4.

High-Performance Computing Provides First Simulation of Abrupt Climate Change

ABSTRACT

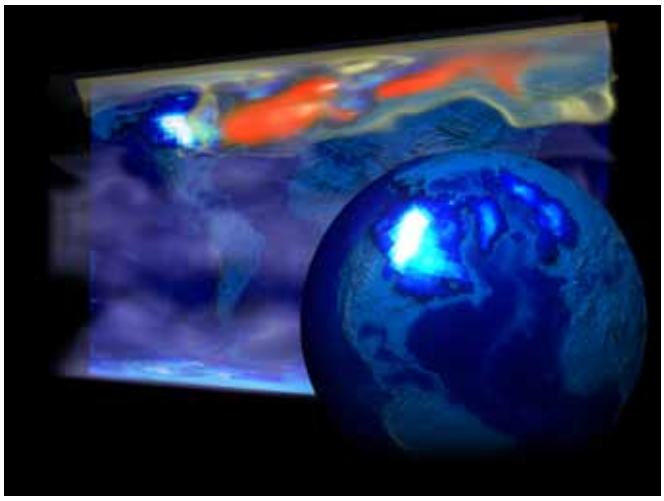
Researchers completed the world's first continuous simulation of 21,000 years of Earth's climate history, from the last glacial maximum to the present. The findings elucidated an episode of abrupt climate change and could provide insight into the fate of ocean circulation in light of continued glacial melting in Greenland and Antarctica.

At DOE's ORNL, one of the world's fastest supercomputers made it possible to simulate abrupt climate change for the first time and shed light on an enigmatic period of natural global warming in Earth's relatively recent history. Zhengyu Liu, director of the University of Wisconsin's Center for Climatic Research, and Bette Otto-Bliesner, an atmospheric scientist and climate modeler at the NCAR, led an interdisciplinary, multi-institutional research group that completed the world's first continuous simulation of 21,000 years of Earth's climate history, from the last glacial maximum to the present, in a state-of-the-art climate model. The unprecedented work was featured in the July 17, 2009, issue of the journal *Science* and provided insight about the causes and effects of global climate change.

In Earth's 4.5-billion-year history, its climate has oscillated between hot and cold. Today our world is relatively cool, resting between ice ages. Variations in planetary orbit, solar output, and volcanic eruptions all change Earth's temperature. Since the Industrial Revolution, however, humans have probably warmed the world faster than has nature. Greenhouse gases we generate by burning fossil fuels and forests will raise the average global temperature 2 to 12 degrees Fahrenheit this century, the IPCC estimates.

Most natural climate change has taken place over thousands or even millions of years. But an episode of abrupt climate change occurred over centuries—possibly decades—during Earth's most recent period of natural global warming, called the Bolling-Allerod warming. Approximately 19,000 years ago, ice sheets started melting in North America and Eurasia. By 17,000 years ago, melting glaciers had dumped enough fresh water into the North Atlantic to stop the overturning ocean circulation, which is driven by density gradients caused by influxes of fresh water and surface heat. This occurrence led to a cooling in Greenland called the Heinrich event 1. The freshwater flux continued on and off until about 14,500 years ago, when it virtually stopped. Greenland's temperature then rose by 27 degrees Fahrenheit over several centuries, and the sea level rose about 16 feet. The cause of this dramatic Bolling-Allerod warming has remained a mystery and source of intense debate.

"Now we are able to simulate these transient events for the first time," said Liu, a professor of atmospheric and oceanic sciences and environmental studies. The research supports a 20-year DOE priority to expand the frontiers of scientific discovery through advanced computation. "It represents so far the most serious validation test of our model's capability for simulating large, abrupt climate changes. This validation is critical for us to assess the model's projection of abrupt changes in the future."



Simulations show deglaciation during the Bolling-Allerod, Earth's most recent period of natural global warming. Image courtesy Jamison Daniel, ORNL

Added Otto-Bliesner, "Several other groups are also working on this type of long simulation, for example, the Bristol University climate modeling group. We want to go further. Our next step is to perform simulations to explore how sensitive the results are to each of the external forcings. In the near future, we will construct isotope-enabled Earth system models to repeat these simulations such that we can compare the model output with proxy records explicitly."

Three-part mechanism for abrupt change

Most climate simulations in comprehensive climate models are discontinuous, amounting to snapshots of century-sized time slices taken every 1,000 years or so. Such simulations are incapable of simulating abrupt transitions occurring on centennial or millennial timescales. Liu and Otto-Bliesner employ petascale supercomputers to stitch together a continuous stream of global climate snapshots and recover the virtual history of global climate in a motion picture representing 21,000 years of data. They use the Community Climate System Model (CCSM), a global climate model that includes coupled interactions among atmosphere, oceans, lands, and sea ice developed with funding from NSF, DOE, and the National Aeronautics and Space Administration (NASA).

Based on insights gleaned from their continuous simulation, Liu and his colleagues propose a novel mechanism to explain

the Bolling-Allerod warming observed in Greenland ice cores. Their three-part mechanism matches the climate record.

First, one-third of the warming, or 9 degrees Fahrenheit, resulted from a 45-parts-per-million increase in the atmospheric concentration of carbon dioxide, the scientists posit. The cause of the carbon dioxide increase, however, is still a topic of active research, Liu said.

Second, another one-third of the warming was due to recovery of oceanic heat transport. When fresh meltwater flowed off the ice sheet, it stopped the overturning ocean current and in turn the warm surface current from low latitudes, leading to a cooling in the North Atlantic and nearby region. When the melting ice sheet was no longer dumping fresh water into the North Atlantic, the region began to heat up.

The last one-third of the temperature rise resulted from an overshoot of the overturning circulation. "Once the glacial melt stopped, the enormous subsurface heat that had accumulated for 3,000 years erupted like a volcano and popped out over decades," Liu hypothesized. "This huge heat flux melted the sea ice and warmed up Greenland."

The 2008 simulations ran on a Cray X1E supercomputer named Phoenix and a faster Cray XT system called Jaguar. The scientists used nearly a million processor hours in 2008 to run one-third of their simulation, from 21,000 years ago—the most recent glacial maximum—to 14,000 years ago—the planet's most recent major period of natural global warming. With 4 million INCITE processor hours allocated on Jaguar for 2009, 2010, and 2011, they completed the simulation, capturing climate from 14,000 years ago to the present. No other research group has successfully simulated such a long period in a comprehensive climate model.

"The unique challenge here is the long duration of simulation, which requires careful model forcing design and extensive sensitivity experiments," Liu said. "Models of this class have never before been run for 10,000 years." As more data become available from such sources as ocean sediments, ice cores, and isotopic analyses, scientists can reduce uncertainty about ancient conditions in their models. To create the most likely conditions for historical meltwater forcing, they can simulate parallel schemes representing 1,000-year periods and select the simulation best resembling observations for their model.

More accurately depicting the past means clearer insights into climate's outlook. "The current forecast predicts the ocean overturning current is likely to weaken but not stop over the next century," Liu said. "However, it remains highly uncertain whether abrupt changes will occur in the next century because of our lack of confidence in the model's capability in simulating abrupt changes. One critical issue is the lack of accurately dated meltwater history just before 14,500 years ago. As such, it remains unclear in the observation if abrupt warming is caused by abrupt termination of the meltwater or abrupt change of the thermohaline system. Our simulation is an important step in assessing the likelihood of predicted abrupt climate changes in the future because it provides a rigorous test of our model against major abrupt changes observed in the recent past."

In 2004 and 2005, climate simulations on DOE supercomputers contributed data to a repository that scientists worldwide accessed to write approximately 300 journal articles. The published articles were cited in the Fourth Assessment Report of the IPCC, which concluded that global warming is definitely happening and humans have probably caused most of the warming since the mid-twentieth century. This transient simulation was the first to explicitly address the issue of abrupt changes and will provide a benchmark for future IPCC reports.

Liu and Otto-Bliesner's simulations may soon find their way into IPCC's data repository and reports as other groups succeed in continuous simulation of past abrupt climate changes and demonstrate the results are reproducible. Meanwhile, Earth's climate continues to prove that change is an eternal constant. Understanding how we affect the rate of change is a grand challenge of our generation. Petascale computing may accelerate answers that in turn inform our policies and guide our actions.

Contributors/Authors

Zhengyu Liu, University of Wisconsin's Center for Climatic Research; Bette Otto-Bliesner, NCAR

Principal Collaborators

The contributors work with Feng He, Anders Carlson, and John Kutzbach, University of Wisconsin–Madison; Esther Brady and Robert Tomas, NCAR; Peter Clark and Edward Brook, Oregon State University; Jean Lynch-Stieglitz, Georgia Tech; William Curry, Woods Hole Oceanographic Institution; David Erickson, ORNL; Robert Jacob, Argonne; and Jun Cheng, Nanjing University of Information Science and Technology.

Funding

The researchers use CCSM, a global climate model that includes coupled interactions among atmosphere, oceans, lands, and sea ice developed with funding from NSF, DOE, and NASA.

Publications

F. He. 2011. "Simulating Transient Climate Evolution of the Last Deglaciation with CCSM3 (TraCE-21K)." PhD dissertation, University of Wisconsin–Madison.

J. Cheng et al. 2010. "Modeling Evidence of North Atlantic Climatic Impact on East Asia." *Chinese Science Bulletin* 55: 3215–3221.

Z. Liu et al. 2009. "Transient Simulation of Last Deglaciation with a New Mechanism for Bolling-Allerod Warming." *Science* 325, no. 5938 (July 17): 310–314.

Supercomputers Predict the Structures of Large Proteins Key in Health

ABSTRACT

Researchers are using Argonne Leadership Computing Facility supercomputers to gain a deeper understanding of protein structure and function. Determining the structures of proteins containing more than 200 amino acids and designing enzymes may illuminate diseases in which proteins may misfold, such as Alzheimer's, and enable design of novel therapeutics.

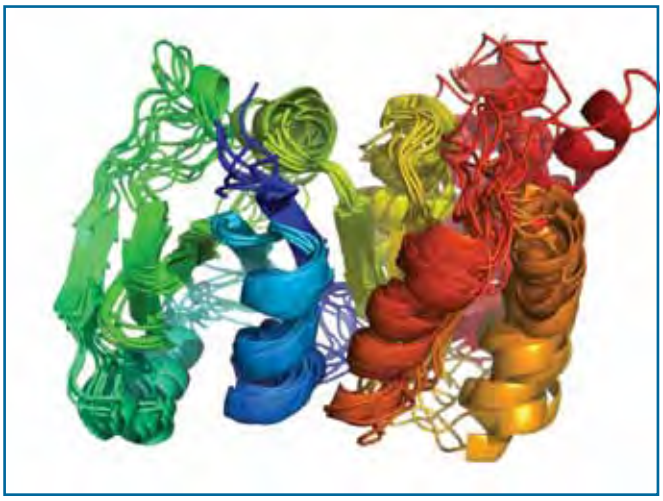
Before the science community can fully comprehend how biological systems work, researchers must develop a deep understanding of proteins: the tiny organic machines that carry out the chemical and biological processes of life.

Amino acids, the building blocks of proteins, are molecules of carbon, hydrogen, nitrogen, and oxygen. Proteins begin life as clusters of amino acids but cannot do their intended work until they fold—that is, collapse from chains into helices and pleated sheets and, later, interlocking 3D configurations. When a protein folds correctly into its favored natural configuration—known as its ground state—it forms its lowest-energy 3D atomic structure. But when protein folding goes wrong, serious repercussions can result. Researchers now believe conditions such as Alzheimer's disease and cystic fibrosis may arise in part from faulty protein folding.

A research team led by David Baker of the University of Washington is using the power of the IBM Blue Gene/P supercomputer at the ALCF to elucidate the rules that govern a protein's folding. What the team's multipronged research uncovers is expected to give scientists a greater understanding of proteins and even equip them to design protein-based enzymes—proteins that increase the rate of chemical reactions—which have many applications, such as for bioremediation, clean energy, biofuels, and therapeutics. "The goal of our research is to develop robust methods for predicting the structures of naturally occurring proteins and to design new proteins with new and useful functions. Leadership computing is critical to these efforts," said Baker.

> In the next few years, our group plans to continue pushing the limits of structure prediction and design using cutting-edge computing resources.
> —David Baker, University of Washington

Armed with limited data, the team recently formulated methods for modeling protein structures and predicting the structure of protein membranes and benchmarked computational strategies for designing proteins with novel functions. Working with information on only amino acid sequences, the team developed Rosetta, a software package of computational algorithms, to design proteins at the atomic scale and predict how they will fold.



Baker's code used a novel NMR methodology run on the ALCF's Intrepid supercomputer to determine the structure of ALG13, an important cellular protein. Image courtesy Oliver Lange

Nuclear magnetic resonance (NMR) spectroscopy, a standard technology for determining protein structures, presents certain limitations. For example, routine NMR applications achieve a maximum protein size of 15 kilodaltons, while most biologically relevant proteins average 30 kilodaltons in size. By applying the Rosetta software, the team has been able to use NMR technology to predict protein size up to 20 kilodaltons. Applying conformational sampling using highly parallel computations on the ALCF's IBM Blue Gene/P supercomputer, researchers are now using NMR technology to draw ever closer to an important breakthrough—determining the protein structures of more than 200 amino acids (20 kilodaltons). These calculations employ up to 32,000 cores and are possible only through the resources provided by the INCITE program.

Another area of the team's research pertains to predicting the structures of membrane proteins essential to many biological functions, including cell stability, bioenergetics, and signal transduction. The majority of drug targets are membrane proteins; however, these protein structures have been difficult to ascertain using conventional methodology. The team adapted the Rosetta de novo method to determine the structure of membrane proteins. For large and complex proteins, the researchers incorporated cryo-electron-microscopy-derived electron density maps into the Rosetta software. This adaptation will equip the team to generate the first-ever high-resolution structures of such membrane proteins.

"In the next few years, our group plans to continue pushing the limits of structure prediction and design using cutting-edge computing resources," Baker remarked.

Making inroads into protein design

Designing novel proteins for use in medical applications—another focus of this research—is one of the most important challenges in structural biology. Novel proteins could help researchers cure diseases and design proteins that can efficiently catalyze medically and industrially useful reactions. For instance, one medical application of the research findings could be to block flu virus infection.

When designing proteins scientists must understand the interactions between them, which play a key role in diverse cellular processes, including immune recognition, host–pathogen interactions, and cell signaling. So far most existing approaches have used in vitro selection of antibodies or other specialized protein "scaffolds." While some have yielded promising therapeutics, they have been labor intensive, relied on serendipity, and sometimes resulted in proteins that are bound to epitopes (molecules that, when introduced into the body, trigger the production of an antibody by the immune system) other than the desired one. By contrast, computational design can target specific regions on a pathogen's surface to block infection.

Besides revealing enzymes important in health and disease, the group's MD codes are also relevant to enzymes crucial for energy production. Research is under way to refine enzyme design methods. For instance, by applying computational protein design methods, the team is engineering *E. coli* to grow with carbon dioxide as the sole carbon source and electricity as the sole source of energy.

The broader implications of this research may prove critical in addressing many of this century's most pressing issues. For example, the research into proteins and their dynamics represents a step in creating biofuels, cleaning up waste, and sequestering carbon. This work advances DOE's mission to transform the scientific understanding of energy and the consequences of its use to advance economic and energy security.

Contributors/Authors

David Baker, University of Washington

Principal Collaborators

All of the following collaborators are affiliated with the University of Washington.

T.J. Brunette, Firas Khatib, and David Kim made ab initio structure prediction possible for proteins over 15 kilodaltons. Oliver Lange and Nikolaos Sgourakis facilitated NMR structure determination for large proteins (greater than 25 kilodaltons). Yifan Song made the calculation of membrane proteins possible using limited NMR and cryo-electron microscopy data. Frank Dimaio made crystallographic phasing possible with template models worse than about 1.5 to 2 angstroms from the native model. Kui Chan, Will Sheffler, and Justin Siegel designed more active catalysts for energy-related applications. Sarel Fleishman, Eric Procko, and Tim Whitehead improved the protein–protein interface design for medical applications. Liz Kellogg and Oliver Lange developed the energy landscape simulation to model entropic conditions around the native state and the active site. T.J. Brunette improved how the search selects where to focus computational resources and how structure diversity is maintained.

Funding

Howard Hughes Medical Institute; Department of Defense, Defense Advanced Research Project Agency; Department of Defense, Defense Threat Reduction Agency; DOE, Advanced Research Projects Agency-Energy; and Department of Health and Human Services, National Institutes of Health

Publications

S. Raman et al. 2010. "NMR Structure Determination for Larger Proteins Using Backbone-Only Data." *Science* 327: 1014–1018.

L. Jiang et al. 2008. "De Novo Computational Design of Retro-Aldol Enzymes." *Science* 319, no.5868: 1387–1391.

D. Röthlisberger et al. 2008. "Kemp Elimination Catalysts by Computational Enzyme Design." *Nature* 453: 190–195.

B. Qian et al. 2007. "High-Resolution Structure Predictions and the Crystallographic Phase Problem." *Nature* 450: 259–264.

Simulations Spur Scientists to Revise Theory of How Stars Explode and a Pulsar Gets Its Spin

ABSTRACT

Using Oak Ridge National Laboratory supercomputers, researchers of core-collapse supernovas showed the exploding star's shock wave may be unstable, drive stellar magnetic fields, and spin the neutron-rich core remaining after the blast to produce a pulsar. The results illuminate how cosmic catastrophes can create and spread elements throughout the universe.

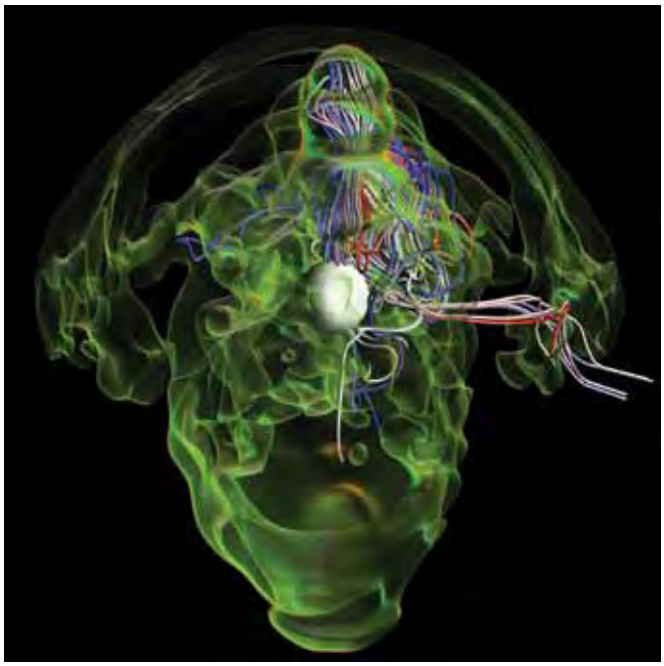
When a supergiant star collapses, its core material condenses into an extremely compact mass that undergoes a rebound. The resulting shock wave sends the matter surrounding the core flying into space and leaves a neutron star at the site of the core's collapse. The shock waves induce further fusion in the matter surrounding the collapsed core. In the process elements are produced that are scattered into the cosmos, along with elements produced throughout the star's lifetime, to form the stuff of new stars and planets.

In a team led by ORNL's Anthony Mezzacappa, John Blondin of North Carolina State University made two revolutionary advances in our understanding of core-collapse supernovas, or the death throes of stars greater than eight solar masses. The results were published in a 2007 issue of the journal *Nature*. The understanding of core-collapse supernovas bears directly on DOE's 20-year priorities to illuminate the origins of matter and energy as well as new forms of nuclear matter at high energy densities and at the extreme limits of stability.

The team's first discovery was that the shock front created by the star's rebounding iron core is unstable when it is stalled by infalling material from the star. This instability is known as the standing accretion shock instability (SASI). The shock front eventually becomes distorted by the SASI and, in 3D simulations, creates two rotating flows—one aligned with but directly below the shock wave and an inner flow that travels in the opposite direction. The result is a coherent slosh.

> The speed of the ORNL supercomputers enabled us to perform the first 3D simulations of an accretion shock that led to these two discoveries.
> —John Blondin, North Carolina State University

Second, Blondin found that the inner flow has enough angular momentum to spin up the neutron star that remains after most of the massive star is blown into space. After a supernova explosion, the remaining core is an object made primarily of neutrons. If that neutron star spins, it becomes what is known as a pulsar. Pulsars beam radiation from their magnetic poles. To an observer watching that beam sweep the sky with each rotation, a pulsar appears to blink like a lighthouse. Before Blondin's SASI discovery, astronomers did not have a workable explanation for how all pulsars get their spins. They assumed they were relics of the spins of the original stars. If that were true, a pulsar would spin much faster than its much larger progenitor, as an ice skater spins faster by pulling in his or her arms. But this explanation accounts for only the fastest observed pulsars. In contrast, Blondin's simulations predict spin periods within the observed range for all pulsars.



Astrophysicists revised theories about supernovas after simulations of supernova shock waves and the discovery of the SASI, and its consequences. Image credit: Dave Pugmire, ORNL

"The speed of the ORNL supercomputers enabled us to perform the first 3D simulations of an accretion shock that led to these two discoveries," Blondin said. "Because the simulations could run in less than a week, rather than months, we were able to run many models to investigate the nature of the SASI, confirm its robustness in the setting of core-collapse supernovae, and study its possible consequences."

New understanding of the universe

The principal source of elements in the universe, core-collapse supernovas provide most of the elements between atomic numbers 8 (oxygen) and 26 (iron) and about half the elements heavier than iron. Therefore, Blondin's discoveries are indispensable to understanding the evolution of the universe and the origins of life.

The SASI is a new piece of supernova theory that has become the framing concept for most current supernova simulations. It not only is key to understanding how the stalled shock front is reenergized and eventually blows most of the star into space but also provides the first explanation for pulsar spin that matches observations. This validation gives researchers confidence they are on their way toward correctly simulating the complex physical mechanisms of a core-collapse supernova.

The counter-rotating currents that may give pulsars their spin had escaped researchers until Blondin was able to perform precision simulations in three dimensions with both sufficient resolution and a well-constructed physical model of a supernova. These spins did not exist in two-dimensional (2D) simulations, which impose an axial symmetry on the exploding star that is not found in nature.

To reach these answers and others, the team led by Mezzacappa developed a sophisticated suite of simulation tools that incorporate state-of-the-art physical theories, high-fidelity numerical solution techniques, parallel algorithms, and efficient and robust software. The tools, which include the CHIMERA and GenASiS scientific application codes, model extremely complex physics, including shock physics, neutrino transport with complex neutrino–matter interactions, magnetohydrodynamics, nuclear fusion, and general relativistic gravity.

The group's recent simulations led by Eirik Endeve of ORNL, with results reported in a 2010 issue of *The Astrophysical Journal*, built on Blondin's earlier work and showed that the driver behind the pulsar spin may also be responsible for the unfathomably strong magnetic fields observed in neutron stars. As the expanding shock wave churns to a halt, matter outside its boundary submerges below the shock, creating vortices that roil the star's magnetic fields. Concurrently running GenASiS on approximately 100,000 of Jaguar's processing cores allowed researchers to execute one of the world's largest simulations of stellar magnetic fields and quickly arrive at this conclusion.

Ultimately, the jackpot in core-collapse supernova research will be a complete explanation of how the collapse of a star's core leads to the explosion that ejects most of its layers. Recent simulations by Mezzacappa's team and others, which include much of the important supernova physics but fewer spatial dimensions, have yielded promising results. However, as yet no model is sufficiently realistic to capture the complexities of these cosmic catastrophes in nature's three dimensions. Whereas earlier high-performance computing systems led to the discovery of the SASI and an explanation of how pulsars get their spins, only using an exascale system—one a thousand times more powerful than present-day petascale systems—will we be able to fully explain how core-collapse supernovas explode and how they produce the elements necessary for life.

Contributors/Authors

John Blondin, North Carolina State University; Anthony Mezzacappa and Eirik Endeve, ORNL

Principal Collaborators

Principal scientific collaborators are Christian Cardall, Raphael Hix, Eric Lingerfelt, and Bronson Messer of ORNL; Reuben Budiardja of the University of Tennessee–Knoxville; and Stephen Bruenn and Pedro Marronetti of Florida Atlantic University. Principal computer science collaborators are Steven Carter, Nageswara Rao, and Ross Toedte of ORNL; Scott Atchley, Micah Beck, and Terry Moore of the University of Tennessee–Knoxville; and Kwan-Liu Ma of the University of California–Davis.

Funding

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Publications

J. Blondin and A. Mezzacappa. 2007. "Pulsar Spins from an Instability in the AccretionShock of Supernovae." *Nature* 445 (January 4): 58–60.

E. Endeve et al. 2010. "Generation of Magnetic Fields by the Stationary Accretion Shock Instability." *The Astrophysical Journal* 713, no. 2 (April 20): 1219–1243.

Scientists Model the Molecular Basis of Parkinson's Disease

ABSTRACT

Supercomputers power the work of researchers studying Parkinson's disease, a neurological disorder that affects more than 2 million people in the United States. Using simulations the team identified the protein responsible for the disorder and is studying its behavior in human membranes, making significant progress toward the development of drugs to treat the disease.

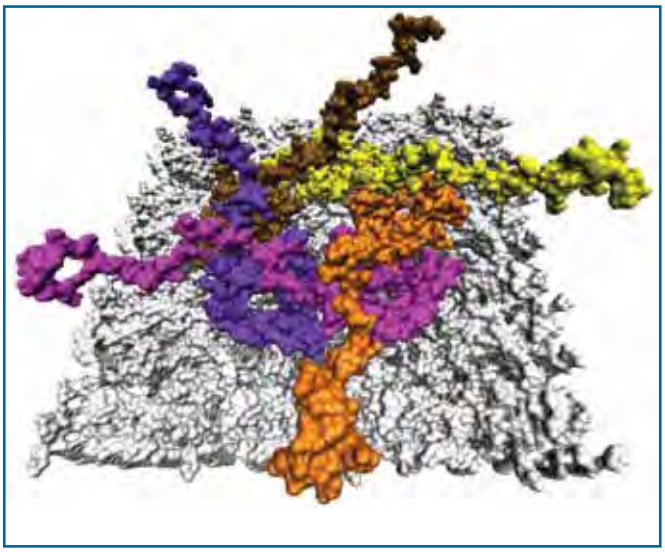
As the second most common neurological disorder in adults, Parkinson's disease has enormous personal and economic impacts. With more than 2 million cases having been diagnosed in the United States alone, this degenerative disease exacts an estimated cost of $25 billion on the nation's economy per year. At present the drugs available to treat Parkinson's disease relieve symptoms but do not provide a cure.

A research team from UCSD is studying the molecular basis of Parkinson's disease and exploring ways to treat it. Under the direction of Igor Tsigelny at UCSD's San Diego Supercomputer Center (SDSC) and Department of Neurosciences, the team has identified alpha-synuclein as the protein responsible for the disease. By evaluating various 3D conformations of the protein, researchers have discovered that the aggregation, or "clumping," of alpha-synuclein protein in the brain can lead to harmful, pore-like structures in human membranes.

The team's multifaceted study seeks to understand why some proteins aggregate and what structural or sequence features may increase their propensity to do so, how proteins penetrate membranes to form pore-like structures, and what role protective molecules play in influencing protein aggregation. In addition, the team is working to identify ways to prevent pores from forming.

> Thanks to the power of supercomputing, we are making major progress in understanding the origins of Parkinson's disease and developing innovative ways to treat it.—Igor Tsigelny, University of California–San Diego

This research has elicited great interest in the scientific community, not only for its potential to halt and treat Parkinson's disease, but also because of its relevance to broader applications. For example, the team's preliminary findings hold significant promise for unlocking the secrets of Alzheimer's and Huntington's diseases, some cancers, and prion protein particles widely believed to cause a number of brain diseases, such as Creutzfeldt-Jakob disease.



UCSD scientists have shown that the aggregation of certain proteins, known as alpha-synuclein, in the brain can lead to harmful, pore-like structures in human membranes. Image courtesy I. F. Tsigelny and Y. Sharikov of UCSD SDSC

By leveraging the high-end power of the Blue Gene/P supercomputer at the ALCF, the team is performing computational modeling of the alpha-synuclein protein.

The supercomputer's power has proved invaluable to researchers in their modeling of MD to uncover the molecular basis of the disease. "The proteins and peptides studies do not have stable conformations, so prolonged molecular dynamics simulations are absolutely necessary to enumerate all possible conformers," explained Tsigelny. "Moreover, the presence of a membrane in simulations makes the system studied very big, in many cases with more than 1 million atoms. Without high-performance computers, these simulations could not be conducted."

In collaboration with the research team, Eliezer Masliah at the UCSD Department of Neurosciences is conducting experimental validations of the modeling and simulation results obtained. To date the correlations between the computational modeling predictions and laboratory experimental results have been encouraging. The team has developed drug-candidate compounds that show promising results in animal studies.

In fact, the findings provide a fertile test bed for identifying possible experimental drugs, that, it is hoped, may ultimately provide a cure for Parkinson's disease. In this regard the computational approach has been particularly successful. The team is modeling alpha-synuclein in specific conformations, creating a number of design templates. Using these templates researchers have created hypothetically designed pharmacophores—groups of atoms whose arrangement in a molecule

triggers certain biological activities. In recent years pharmacophore modeling has enabled other research teams to develop effective drugs to treat many conditions.

Through this modeling Tsigelny's team has produced three drug candidates with high potential for treating Parkinson's disease by stopping or preventing pore formation. Each theoretical design was tested in the laboratory and found to be effective. Patents for all three drug candidates are pending. The team continues to identify additional compounds for drugs that are high performers in inhibiting protein aggregation and confirm this quality through biomedical experimentation.

"Thanks to the power of supercomputing, we are making major progress in understanding the origins of Parkinson's disease and developing innovative ways to treat it," stated Tsigelny.

Research yields another promising application

The team's exploration of pore formation in bacterial membranes may also yield answers to problems associated with environmental waste by reducing radionuclides—atoms that emit harmful radioactivity—and eliminating environmental waste through absorption. Working with scientists in Ukraine, the team is organizing an initiative in which it will conduct experimental validation of efforts to clean radionuclides from water in Chernobyl.

To this end the researchers are building a program package for the study of proteins' aggregation and interaction with membranes. This set of programs will help equip future research teams to study other biomedical and environmental problems in which the membrane contact of proteins is involved. "Our simulations have shown the clear creation of annular protein aggregates that can penetrate to the bacterial membranes and create the pores in them," said Tsigelny. "Such pores are open for absorption of radionuclides. We are working with various mutations of microcid proteins [enzymes that have antibacterial properties when exposed to glucose and oxygen] to obtain a controllable set of proteins."

In the future the research team will continue its comprehensive investigation of alpha-synuclein penetration into the membrane, including a deeper study of aggregation and pore creation. It has started to work with multicomponent membranes that are much closer to real cell membranes than the 1-palmitoyl-2-oleoyl-phosphatidylcholine ones used before. The researchers will also begin to study the beta-amyloid protein, known to be responsible for Alzheimer's disease, and explore a set of known mutations of the alpha-synuclein and beta-amyloid proteins. Because of their work, the millions who suffer from degenerative neurological disorders are being given new hope.

Contributors/Authors

Igor Tsigelny, SDSC and Department of Neurosciences, UCSD and Eliezer Masliah, Department of Neurosciences, UCSD

Funding

SDSC and UCSD, Department of Neurosciences

Publications

L. Seung-Jae et al. 2010. "Cell-to-Cell Transmission of Non-prion Protein Aggregates." *Nature Reviews Neurology* 6 (December): 702–706.

I. Tsigelny et al. 2008. "Mechanism of Alpha-synuclein Oligomerization and Membrane Interaction: Theoretical Approach to Unstructured Proteins Studies." *Nanomedicine* 4, no. 4 (December): 350–357.

L. Crews et al. 2009. "Role of Synucleins in Alzheimer's Disease." *Neurotox Res.* 16, no. 3 (October): 306–317.

Y. Sharikov et al. 2008. "MAPAS: A Tool for Predicting Membrane-Contacting Protein Surfaces." *Nature Methods* 5, no.119 (February): 119–120.

Unprecedented Simulation Lessens the Risk of Combustion Instabilities in Turbines

ABSTRACT

Research employing Argonne Leadership Computing Facility supercomputers aims to improve knowledge of two-phase flows (for example, fuel in gaseous and liquid forms) and their combustion in gas turbines. This understanding will allow a better assessment of the impacts of new designs and fuels on the efficiency of helicopter and airplane engines.

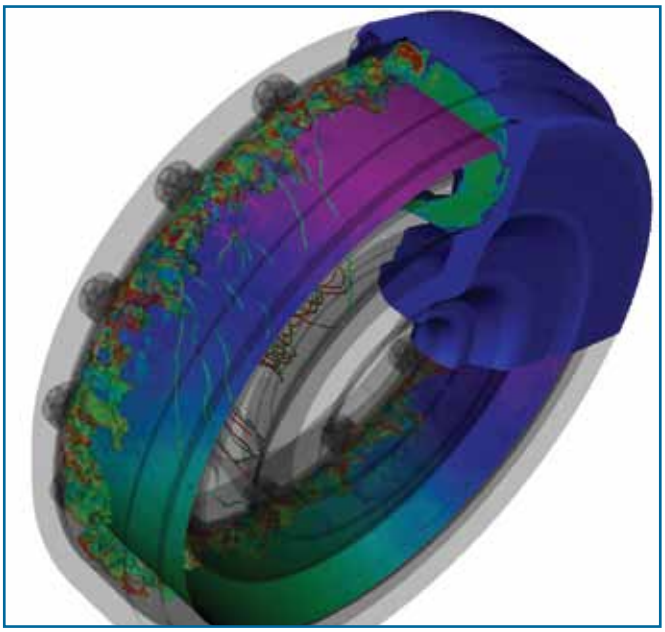
Today more than 80 percent of the energy people use is consumed through the burning of fossil fuels (that is, through sustained, turbulent combustion). If engineers could fully understand what effects design or fuel changes would have on combustion engines before building and testing prototypes, they could save both time and money and make more rapid progress toward developing highly energy-efficient and safer engines for vehicles of the future. Simulations at the ALCF are allowing one team of researchers to do just that.

The team, led by Thierry Poinsot of the Center for Research and Formation for Advanced Scientific Computations (CERFACS), is using LES techniques to track flows of fuel and air as the turbulent mixture ignites and burns. By modeling the reacting flow at scales at which engine components can exert effects—from hundredths to millionths of a meter—LES techniques offer levels of precision never before attained.

"LES techniques give us unprecedented precision in modeling unsteady turbulent combustion in practical components, such as the combustion chamber of an aircraft, but they require significant computing power," said Poinsot. "In that sense, massively parallel machines are the real heart of LES for reacting flows."

Currently, CERFACS researchers are focusing on LESs of gas turbine engines. They have developed a simulation code using unstructured grids that can be applied to any geometry, not just square domains, as was the case for most CFD methods before 2005. Using unstructured grids for CFD allows researchers to take into account the complex shapes of actual combustors. It also leads to efficient domain decomposition and high parallel performances on machines like Intrepid, the IBM Blue Gene/P supercomputer at the ALCF. By using this code, the team has been able to perform the largest LES conducted to date of a full-sized commercial combustion chamber used in an existing helicopter engine.

The computation was ten times larger than any previous simulation and performed on 330 million grid cells. At each point ten variables were solved (for velocities, density, temperature, and chemical species) over 100,000 time iterations. The production runs used more than 16,000 cores of Intrepid, corresponding to 10 percent of the complete system at that time.



Fields of temperature and pressure are shown in a 330-million-elements simulation of a complete helicopter combustion chamber performed on the IBM Blue Gene/P at the ALCF. Image courtesy Pierre Wolf, Turbomeca and CERFACS

The total amount of data generated during the simulation was on the order of 10^{15} numbers and required 6 months for analysis. CERFACS, Argonne, and Stanford University collaborated on the analysis during the Stanford Center for Turbulence Research (CTR) 2010 Summer Program.

Overall, the team's simulations have confirmed the nature of the unstable modes observed in the helicopter engine. In annular combustion chambers (a common configuration in aero engines), the two phenomena that most often couple and can lead to instabilities and major problems, including engine explosion or loss of control, are acoustic modes and unsteady combustion. The acoustic modes in these chambers are usually azimuthal modes in which sound waves travel in the azimuthal direction in the annular chamber. These waves couple with unsteady flame movements and can lead to instabilities. CERFACS' LES has confirmed the presence of these modes in actual engines and helped engineers modify designs to control them.

"The impact of the INCITE project on our research is essential because it brings capacities that were simply not available up to now and allows us to compute commercial engines and not only laboratory-simplified setups," Poinsot asserted.

The team's work addresses DOE's mission to improve energy security and efficiency and its 20-year priority to expand the frontiers of scientific discovery through leadership-class computing.

Combustion simulations extended to liquid fuels

The researchers have now extended the computational capabilities deployed in previous studies of combustion of gases to those of liquid fuels in gas turbines.

Bringing LES methodology to combustion devices represents a huge step in computing technology and modeling. In addition to tracking the gaseous flow, the simulation must take into account the movement of millions of fuel droplets that evaporate before burning. This approach allows the researchers to tackle challenging issues such as ignition of the fuel cloud, quenching, or instabilities encountered in gas turbine engines undergoing combustion as well as create designs that optimize performance and safety. These issues are paramount to fully understanding what happens in airplane and helicopter engines and in gas turbines used in power generation. The significant development of the LES code carried out at CERFACS since 2007 now enables the researchers to advance toward the full numerical engine test bench. A complete software code would allow engineers to simulate the engine before building it and assess the impact of any change on any parameter of the combustion inside the engine, such as replacing kerosene with a biofuel or modifying the injector of a combustor. Such simulations are mandatory to replace experiments (which are very costly for gas turbines), explore multiple designs, and determine which designs are optimal and safe before they are built.

To perform their computations, the researchers are using CERFACS' LES code AVBP, which has demonstrated extremely good scalability on up to 16,384 cores on diverse architectures. They are currently extending this performance to tens of thousands of cores.

> The impact of the INCITE project on our research is essential because it brings capacities that were simply not available up to now and allows us to compute commercial engines and not only laboratory-simplified setups.—Thierry Poinsot, Center for Research and Formation for Advanced Scientific Computations

The researchers simulated combustion in turbines of two fuel phases—gaseous and liquid. They then compared LES results with laboratory combustion experiments performed on turbines to validate that the simulation results matched their observations. Notably, the effects of mesh refinement, which allows researchers to home in on an area of interest with increased resolution, were validated during Stanford CTR's Summer Program. The influence of the number of grid cells on the LES output was also tested using a simpler, two-phase-flow single burner with three levels of refinement (4-, 8-, and 16-million elements). The results have allowed researchers to identify the structure of the unstable modes appearing in the engine and confirmed the nature of the modes experimentally observed in the real engine. These modes are now clearly recognized as azimuthal. Acoustic waves propagate in clockwise and counterclockwise directions in the annular chamber and interact with the flames present in each burner.

Combustion instabilities are an important area into which LES techniques provide insight. The science produced by the simulation has led to an increased understanding of azimuthal combustion instabilities, including characterization of their structure. Previously scientists thought the structure was solely rotating or stationary in nature, but it is now believed to be a hybrid of the two with a very slow, rotating component. This mode is the result of the superposition of an acoustic wave turning in a clockwise direction and a wave turning in a counterclockwise direction. The two waves have slightly different speeds and amplitudes, so their superposition leads to a complex pattern in which points of maximum pressure oscillation turn slowly at a speed that is the mean azimuthal flow convection velocity in the chamber. As new simulations generate more insights into the nature of combustion instabililties, the ongoing work will lead to new strategies on how to prevent such instabilities—and possibly even remove them from current systems.

Contributors/Authors

Thierry Poinsot, CERFACS

Principal Collaborators

Gabriel Staffelbach is a senior researcher at CERFACS and oversees all the developments in the AVBP code at the center. He collaborates directly with ALCF experts to improve AVBP performances on the BlueGene/P system. Ramesh Balakrishnan is a computational scientist at the ALCF. He also works with AVBP and interacted with CERFACS during Stanford's CTR Summer Program in 2010.

Funding

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Publications

M. Sanjose et al. 2011. "Fuel Injection Model for Euler-Euler and Euler-Lagrange Large-Eddy Simulations of an Evaporating Spray Inside an Aeronautical Combustor." *International Journal of Multiphase Flow* 37: 514–529.

P. Wolf et al. 2010. "Azimuthal Instabilities in Annular Combustion Chambers." *Proceedings of the Summer Program, Center for Turbulence Research,* NASA Ames, Stanford University.

P. Wolf et al. 2009. "Massively Parallel LES of Azimuthal Thermo-acoustic Instabilities in Annular Gas Turbines." *Comptes Rendus de l'Académie des Sciences – Mécanique* 337, no. 6–7: 385–394.

Computational Scientists Help Superconductors Find the Path of Least Resistance

ABSTRACT

Superconducting materials are key to eventually developing technologies that save energy in power cables, electric vehicles and trains, and electric machinery. A team is using the Oak Ridge Leadership Computing Facility to perform high-end simulations of cuprate high-temperature superconductors to understand, predict, and optimize their complex behavior and help accelerate their development.

A team led by Thomas Schulthess of ORNL, Eidgenössische Technische Hochschule Zürich (ETH Zürich), and the Swiss National Supercomputing Center studies thin layers of copper and oxygen sandwiched between layers of insulating material. These superconducting cuprates may someday revolutionize particle physics, transportation, and medical diagnostics.

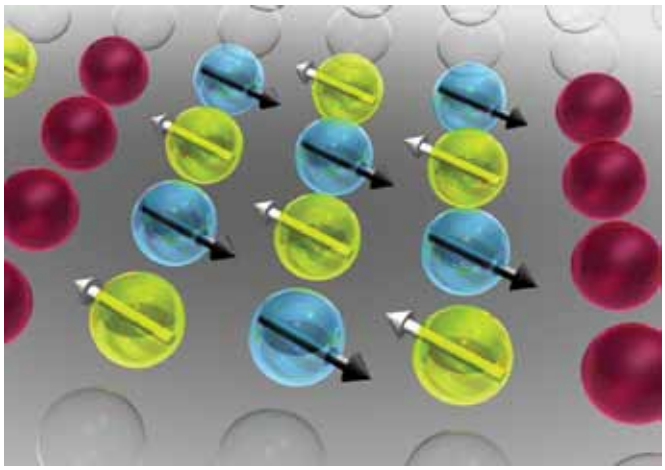
Using ORNL's Cray XT5 Jaguar system, Schulthess and colleagues work from the perspective of individual atoms and electrons to evaluate the effect of disorder among electrons in the system. The team verified the superconducting properties of a promising material composed of lanthanum, barium, copper, and oxygen (LaBaCuO) and published its findings June 16, 2010, in the journal *Physical Review Letters*.

Another paper, which described how the team's DCA++ application was used to solve the 2D Hubbard model, earned a Gordon Bell Prize in 2008 for the world's fastest scientific computing application. In 2010 an honorable mention in the Gordon Bell competition went to Anton Kozhevnikov and Schulthess of ETH Zürich and Adolfo G. Eguiluz of the University of Tennessee–Knoxville for reaching 1.3 petaflops with the Dynamic Response Code application while making full use of Jaguar's 224,256 processing cores to solve the Schrödinger equation from first principles for electronic systems while minimizing simplifying assumptions.

"Petascale computing allows us to think of predicting the properties of unconventional superconductors," said ORNL's Thomas Maier, a physicist on Schulthess's team. "Because of their complexity, previous studies have been limited to simple models. The recent advances in computational hardware have allowed us to make simulations more and more realistic."

Superconducting materials conduct electricity without loss of energy, but they do so only at extremely low temperatures. So far the highest temperature at which a known material transitions into a superconducting state is only 135 Kelvin—no warmer than −216 degrees Fahrenheit.

The earliest superconductors had to be kept below 20 Kelvin (−424 degrees Fahrenheit) and were cooled with liquid helium—a very expensive process. Later materials remained superconducting above liquid nitrogen's boiling point of 77 Kelvin (−321 degrees Fahrenheit), making their use less expensive. The discovery of a room-temperature superconductor would revolutionize power transmission and make energy use ultraefficient.



In a lanthanum-barium-copper-oxygen material, superconductance is good in two dimensions but bad in three. An eight-by-four-atom cluster represents the high-temperature superconductor, with red balls indicating "stripes" of atoms with missing electrons and blue and green balls standing for atoms with alternating electron spins. Image courtesy Jeremy Meredith, ORNL

The nanoscience research of Schulthess and his colleagues, featured in *Breakthroughs 2008*, aligns with a 20-year priority for DOE to construct revolutionary new materials. It supports DOE's science mission and has the potential to support its energy mission, especially energy efficiency, if the full potential of room-temperature superconductors is realized.

Two-dimensional superconductor

Researchers develop new superconducting cuprates by varying insulating layers, which in turn affects the conducting copper-oxygen layer by removing electrons from it (the places where electrons used to be are called holes). This manipulation potentially encourages remaining electrons to join into Cooper pairs, which can carry a current without resistance.

"The material becomes superconducting if you pull out enough electrons from the planes," noted Maier. "You have to do so many substitutions, then the material becomes superconducting. It starts out superconducting at a very low temperature, but once you substitute more and more material in between there, your transition temperature goes up, reaches a maximum temperature, and then goes down again."

A dopant is added to the insulator until the cuprate reaches its highest possible transition temperature; this recipe is known

as optimal doping. In most cuprates optimal doping pulls between 15 and 20 percent of the electrons from the conducting copper-oxygen layer. Generally holes are scattered more or less randomly throughout the layer; however, when barium is substituted for one-eighth of the lanthanum in a lanthanum-copper-oxygen cuprate, the holes line up in stripes.

"Early experiments showed striping at one-eighth doping and saw that transition temperature went way down, and they concluded that striping was bad," Maier explained. "That was the common wisdom until recently, when two independent experiments—one performed at Brookhaven National Laboratory, the other by Brookhaven, Lawrence Berkeley National Laboratory, and Cornell University—showed that if you look at properties other than transition temperature, you find, for instance, that the pairing gap, which tells you how strongly these electrons are bound into Cooper pairs, is highest at this doping."

These experiments also showed that resistance in this material drops at a much higher temperature if you look at single layers of atoms. It was this result that Schulthess's team was able to computationally verify using the 2D Hubbard model. This model was the most promising for describing high-temperature superconductivity in materials, but its complex equations could not be solved for a large enough set of atoms to model a realistic superconductor. That changed in 2005 when scientists, including members of this team, used the terascale Cray X1E supercomputer at ORNL to solve the 2D Hubbard model and present evidence that it predicts high-temperature superconductivity.

The team's recent results showed the superconducting performance of striped LaBaCuO is excellent when modeled in two dimensions. Some might view a material's stellar performance in two dimensions as nothing more than a fascinating curiosity with no practical value. After all, the real world takes place in three dimensions. But manufacturing technology can lay down layers so thin they are essentially 2D. The transition temperature of the striped LaBaCuO in three dimensions, however, is very low because the stripes of adjacent layers don't line up and the layers are electronically decoupled, Maier noted.

"With recent advances in quantum engineering, one might be able to structure a system like this in the near future. It's not possible yet, but what can be done is to grow these systems layer by layer," Maier said. Researchers could put different dopants in different layers and tune properties layer by layer.

To simulate the effect of disorder on the system, the group used a cluster of 16 atoms, with atoms beyond the boundary represented by an average field. Such a cluster has more than 65,000 possible disorder configurations (i.e., 2^{16}), but the team chose 128 arrangements as a representative sample. To simulate the striped state of LaBaCuO, the team had to simulate a larger cluster of atoms—32—but included only one configuration.

The team performed these simulations as part of the Jaguar system's Early Petascale Science program. Maier said DCA++ ran with nearly the same performance as it had during the Gordon Bell competition and managed about 85 percent efficiency on about 65,000 processing cores.

In the future the team will apply its calculations to iron-based high-temperature superconductors, discovered in 2008. Maier said these superconductors will be far more challenging to simulate than cuprates.

"In the cuprates there is really only one orbital where the action is going on, so we only have to take into account one orbital in the models we are using," Maier noted. Understanding the iron-based superconductors requires modeling five orbitals of the iron that are all active. "It makes it a lot harder," he said.

By allowing for more realistic simulations, supercomputers speed the day when scientists can computationally predict and design the novel materials that could form the basis of tomorrow's ultraefficient electric grids.

Contributors/Authors

Thomas Schulthess, ORNL, ETH Zürich, and Swiss National Supercomputing Center

Principal Collaborators

The team includes Gonzalo Alvarez, Paul Kent, and Thomas Maier, ORNL; Mark Jarrell, Louisiana State University; Alexandru Macridin, University of Cincinnati; Douglas Scalapino, University of California–Santa Barbara; Didier Poilblanc, Laboratoire de Physique Théorique, Centre National de la Recherche Scientifique, and Université de Toulouse.

Funding

DOE Office of Science BES and ETH Zürich

Publications

T. Maier et al. 2010. "Dynamic Cluster Quantum Monte Carlo Simulations of a Two-Dimensional Hubbard Model with Stripelike Charge-Density-Wave Modulations: Interplay between Inhomogeneities and the Superconducting State." *Physical Review Letters* 104, no. 24: 247001.

T. Maier, D. Poilblanc, and D. Scalapino. 2008. "Dynamics of the Pairing Interaction in the Hubbard and t-J Models of High-Temperature Superconductors." *Physical Review Letters* 100, no. 23: 237001.

P. Kent et al. 2008. "Combined Density Functional and Dynamical Cluster Quantum Monte Carlo Calculations of the Three-Band Hubbard Model for Hole-Doped Cuprate Superconductors." *Physical Review B* 78, no. 3: 035132.

G. Alvarez et al. 2008. "New Algorithm to Enable 400+ TFlop/s Sustained Performance in Simulations of Disorder Effects in High-Tc Superconductors." *Proceedings of the ACM/IEEE Conference on Supercomputing 2008, Austin, Texas,* Article 61.

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Supercomputers Simulate the Molecular Machines That Replicate and Repair DNA

ABSTRACT

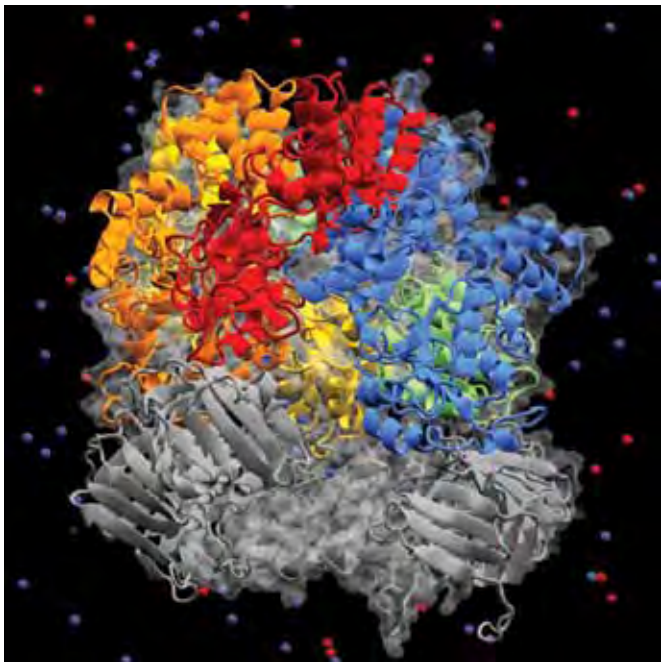
Using the Jaguar supercomputer, scientists model the molecular machines that faithfully duplicate genetic material during cell division. Understanding the role of molecular machines in health and disease may allow exploitation of features that differ among plants, animals, viruses, and bacteria and enable creation of novel drugs with few side effects.

Imagine you are an astronaut. A piece of space junk has cut a gash into the side of the space station, and you have been tasked with repairing the damage. Your spacesuit is equipped with a clamp, which you open, slide onto a tether connecting you to the space station, and close. Then you move to the far end of the gash and begin applying composite material to fill the holes. You glide along the gash making repairs until you are done.

DNA replication, modification, and repair happen in a similar way. That's what groundbreaking biochemical simulations run on one of the world's fastest supercomputers have revealed. Ivaylo Ivanov of Georgia State University, John Tainer of the Scripps Research Institute, and J. Andrew McCammon of UCSD used Jaguar, a Cray XT HPC system at ORNL, to elucidate the mechanism by which accessory proteins, called sliding clamps, are loaded onto DNA strands and coordinate enzymes that enable gene repair or replication. Their findings inspire a new approach for attacking diverse diseases and align with a goal that DOE ranks highly among its 20-year priorities—harnessing the molecular machines of life for energy, the environment, and human health.

"This research has direct bearing on understanding the molecular basis of genetic integrity and the loss of this integrity in cancer and degenerative diseases," Ivanov said. The project focused on the clamp-loading cycle in eukaryotes—or plants, animals, and other organisms whose genetic material is enclosed in a nuclear membrane. Prokaryotes, such as bacteria, whose genes are not compartmentalized, also have a molecular machine to load clamps, but it works a little differently. Viruses, on the other hand, do not have their own clamp loaders but instead co-opt the replication machinery of their hosts.

So how does the molecular machine work in a eukaryote? The researchers revealed that a clamp loader (replication factor C) places a doughnut-shaped sliding clamp (proliferating cell nuclear antigen, or PCNA) onto DNA. The clamp loader first binds to the clamp to activate its opening with energy from adenosine triphosphate (ATP). Protein secondary structures, or beta sheets, at the junctures of the clamp's three subunits, separate at one juncture. A complex made up of the open clamp and the clamp loader then encircles primer-template DNA,



Supercomputers at the OLCF illuminate the workings of the molecular machinery that opens and loads sliding clamps onto DNA. These clamps play vital roles in both DNA replication and repair. Here the clamp loader (with its subunits shown in blue, green, yellow, orange, and red) is depicted in complex with a ring-open sliding clamp (shown in gray) and counterions (spheres). Image courtesy Ivaylo Ivanov of Georgia State University and Mike Matheson of ORNL

which is double stranded in one region and single stranded in another. Again activated by ATP, the clamp closes and is now free to slide along the DNA strand and coordinate enzymes needed for replication and repair.

These sliding clamps and clamp loaders are part of the replisome—the molecular machinery responsible for the faithful duplication of the genetic material during cell division. "The replisome is very complex and dynamic, with interchanging parts. It's an incredibly challenging system to understand," explained Ivanov. "Simulating just a few of its constituent parts—the clamp/clamp loader assembly—required a system of more than 300,000 atoms. To make progress simulating the system in a reasonable amount of time, we needed access to large-scale computing."

An allocation of supercomputing time through the INCITE program allowed the researchers to run NAMD, an MD code. The work consumed more than 2 million processor hours on the Jaguar XT4 and XT5 components in 2009 and 2010, taking a few months of total computing time. Using the kind of machine on which NAMD is usually run, a single simulation continuously running would have taken years.

Master coordinator

In DNA replication the clamp slides along a strand of genetic material made of building blocks called nucleotides. Nucleotides differ only in the type of base they carry, so bases are what determine the genetic message. Enzymes called polymerases catalyze the formation of a new DNA strand from an existing DNA template. The association of the sliding clamps with polymerases significantly increases the efficiency of strand replication, as it prevents polymerases from falling off the DNA and makes sure replication continues uninterrupted. Polymerases iteratively add one of four bases to DNA strands until they have strung together thousands of them.

> Simulating just a few of its constituent parts—the clamp/clamp loader assembly—required a system of more than 300,000 atoms. To make progress simulating the system in a reasonable amount of time, we needed access to large-scale computing.— Ivaylo Ivanov, Georgia State University

In DNA repair the sliding clamp serves as the master coordinator of the cellular response to genetic damage. A number of proteins, such as cell cycle checkpoint inhibitors or DNA repair enzymes, attach themselves to the clamp to perform their functions. In this capacity the role of the clamp is to orchestrate a variety of DNA modification processes by recruiting crucial players to the replication fork, a structure in which double-stranded DNA gives rise to single-stranded prongs that act as templates for making new DNA.

Given the dual function of PCNA in replication and repair, it is not surprising that this clamp has been implicated in diseases accompanied by excessive replication and unchecked cell growth, such as cancer. PCNA modifications are key in determining the fate of the replication fork and, ultimately, both tumor progression and treatment outcome. Therefore, PCNA has been used as a diagnostic and prognostic tool (biomarker) for cancer.

Most studies of DNA replication have focused on polymerases. Gaining a better understanding of the replisome, however, may shift the spotlight. "Instead of just focusing on polymerase, we can interfere with many different components within this complex machinery," Ivanov said. "That may allow new drug targets to be developed for hyperproliferative diseases such as cancer."

Improved understanding of the replisome may make it possible to exploit differences among organisms as diverse as viruses, bacteria, plants, and animals. Although clamp loaders from different kingdoms of life share many architectural features, significant mechanistic differences exist, specifically in the ways ATP is used. Drugs targeted to the clamp loader could selectively inhibit replication of viral DNA in diseases such as chickenpox, herpes, and AIDS without interfering with DNA replication in normal human cells. Similarly, in processes with increased DNA replication, such as cancer, inhibiting clamp loading might produce therapeutic effects without unwanted side effects.

In the future Ivanov and his colleagues will study mechanisms of alternative clamps such as a PCNA-related protein complex that signals the cell to arrest division upon detection of DNA damage. Ultimately the researchers, fueled by enthusiasm at the therapeutic prospects, want to demystify the entire clamp-loading cycle.

Contributors/Authors

Ivaylo Ivanov, Georgia State University; John Tainer, Scripps Research Institute; J. Andrew McCammon, UCSD

Principal Collaborators

The contributors work with Carlo Guardiani, a computational scientist from the University of Florence, on the biomechanics of sliding clamps. Together they apply advanced simulation techniques to elucidate the mechanism of subunit interface disruption in PCNA and the 9-1-1 clamp. Susan Tsutakawa, a structural biologist at LBNL, has worked closely with them on the project and made invaluable contributions to the joint computational/experimental effort to understand the biology of sliding clamps. Specifically, she has carried out small-angle X-ray scattering experiments validating the simulation results on the mode of association between PCNA and covalently bound ubiquitin. Computational chemist Xiaolin Cheng of ORNL has provided helpful input and interactions, specifically with regard to simulations of DNA repair proteins in the base excision repair pathway, and has also worked with Ivanov on simulations of ligand-gated ion channels.

Funding

Howard Hughes Medical Institute and NSF Center for Theoretical Biological Physics

Publications

S. Fritsch et al. 2011. "Ion Selectivity Mechanism in a Bacterial Pentameric Ligand Gated Ion Channel." *Biophysical Journal* 100: 390–398.

J.A. Tainer, J.A. McCammon, and I. Ivanov. 2010. "Recognition of the Ring-Opened State of Proliferating Cell Nuclear Antigen by Replication Factor C Promotes Eukaryotic Clamp-Loading." *Journal of the American Chemical Society* 132, no. 21 (May 10): 7372–7378.

X.L. Cheng et al. 2009. "Molecular-Dynamics Simulations of ELIC—A Prokaryotic Homologue of the Nicotinic Acetylcholine Receptor." *Biophysical Journal* 96. no. 11 (June 3): 4502–4513.

R.E. Amaro et al. 2009. "Characterizing Loop Dynamics and Ligand Recognition in Human- and Avian-Type Influenza Neuraminidases via Generalized Born Molecular Dynamics and End-Point Free Energy Calculations." *Journal of the American Chemical Society* 131, no. 13 (April 8): 4702–4709.

Supercomputing Models Help Scientists Better Understand Carbon Sequestration

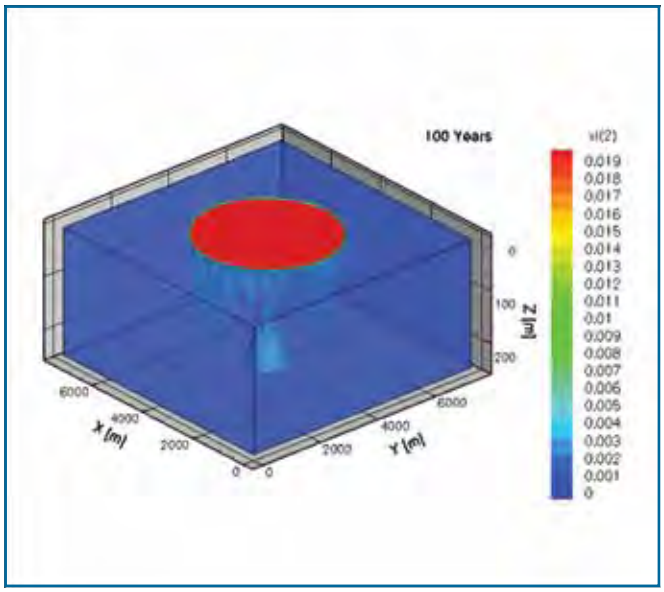
ABSTRACT

Using Oak Ridge National Laboratory's Jaguar supercomputer, researchers are simulating carbon sequestration to ameliorate the harmful effects of emissions from coal burning. Sequestration injects the greenhouse gas CO_2 into a deep saline aquifer in hopes that it will spread under a layer of impermeable rock and dissolve into surrounding brine.

Even as we develop promising energy sources such as solar power, biofuels, and nuclear energy, we face the prospect of being tethered for some time to the old energy sources—primarily fossil fuels such as coal and oil.

One proposal for mitigating the effect of coal power on Earth's climate involves separating carbon dioxide—or CO_2—from power plant emissions and pumping it deep underground, where it can remain indefinitely dissolved in the groundwater or converted into a solid form of carbonate minerals.

A team of researchers led by Peter Lichtner of Los Alamos National Laboratory (LANL) is using the OLCF's Jaguar supercomputer to simulate this process, known as carbon sequestration, searching for ways to maximize the benefits and avoid potential drawbacks.



The simulation illustrates fingering of CO_2 dissolved in brine at an elapsed time of 300 years. CO_2 is injected at a rate of 1 megaton per year for 20 years at a depth of 50 meters, corresponding to roughly 75 percent of the CO_2 produced by a 1,000-megawatt gas-fired power plant in 20 years. The color code represents moles of CO_2 per total moles of water and CO_2. Image courtesy Peter Lichtner, LANL, and Chuan Lu, INL

"Jaguar is essential for carrying out petascale simulations of large basin-scale computational domains on the order of hundreds of kilometers—such as the Illinois basin—to evaluate their potential for storing CO_2," according to Lichtner. The team conducted simulations using a DOE ASCR code, PFLOTRAN. This research directly supports DOE's 20-year priorities to expand the broad frontiers of scientific discovery through the power of advanced computation and to aid in the design of new technologies using principles of biological and physical systems that offer new solutions for challenges to environmental cleanup.

Coal is abundant in the United States, but its use for power causes a variety of serious problems, one of which is that coal-fired power plants spew CO_2 into the air. While carbon sequestration can't handle all man-made sources of CO_2 (cars, airplanes, etc.), it could be used specifically to reduce emissions from large coal-fired power plants throughout the nation.

The process Lichtner's team simulated involves injecting CO_2 into a saline aquifer 1 to 2 kilometers below the surface. If all goes according to plan, it would spread out under a layer of impermeable rock and dissolve into the surrounding brine.

The CO_2 would be pumped in a state known as a supercritical phase—in some ways like a liquid and in others like a gas—that occurs when it is kept above 120 degrees Fahrenheit and more than 100 times atmospheric pressure. The heat and pressure naturally present deep underground would keep the CO_2 in that state, according to Lichtner.

At this point in the investigation of carbon sequestration, there are many unknowns about the effects of pushing CO_2 underground. Despite these unknowns, though, supercomputers are able to provide scientists with a fundamental understanding of the interactions between CO_2 and the underground environment before experiments are conducted. With new understandings about the possible ramifications of carbon sequestration, scientists can improve techniques that will boost the chances of making this a sustainable and cost-effective answer to reducing levels of atmospheric CO_2.

Addressing the unknowns

The rate at which CO_2 dissolves is critical to the success of carbon sequestration. When it is first injected in the ground, the CO_2 pushes the brine out of place. Once the CO_2 dissolves, however, it adds little to the volume of the brine, which can then move back into place.

"The problem is that we're talking about injecting huge amounts of CO_2 by volume," Lichtner explained. "If you were injecting it into a deep saline aquifer, for example, you would initially have to displace the brine that was present, and then the question

is, 'Where does that go?' It's a race against time how rapidly this CO_2 will dissipate."

Lichtner's team is investigating a process known as fingering that speeds the rate at which the CO_2 dissolves. Brine in which CO_2 has been dissolved is heavier than unsaturated brine. Local overdensities of this heavier, saturated brine result in the formation of fingers, which sink into the lighter brine below. This fingering serves to increase the surface area between the heavier and lighter fluids and speeds the dissolution of the supercritical CO_2 into the brine.

"As long as the supercritical phase still exists, it presents a hazard to people living on the surface," Lichtner said, "because it could escape through fractures, abandoned boreholes, or plugged boreholes that leak. And so the rate of dissipation is important to understand to know how rapidly you can get rid of this supercritical phase."

> Jaguar is essential for carrying out petascale simulations of large basin-scale computational domains on the order of hundreds of kilometers—such as the Illinois basin—to evaluate their potential for storing CO_2.—Peter Lichtner, Los Alamos National Laboratory

Another issue under investigation focuses not so much on the rate at which CO_2 dissolves, but rather on the changes this process brings to the aquifer itself. As Lichtner explained, CO_2 produces carbonic acid, which in turn lowers the pH of the brine. This acidification could speed the reaction between the newly acidic brine and surrounding minerals and potentially release contaminants into the environment that would not otherwise be present.

Lichtner's team is simulating carbon sequestration using the PFLOTRAN application. PFLOTRAN is a multiphase, multicomponent reactive flow and transport code that can trace the evolution of multiple constituents through a variety of reactive environments. Chuan Lu of Idaho National Laboratory (INL) developed the supercritical CO_2 implementation in PFLOTRAN while working with Lichtner as a postdoctoral researcher at LANL. Lichtner and his team have shown that PFLOTRAN can handle grids on the order of a billion cells—an unprecedentedly large number for a groundwater simulation. Nevertheless, each cell in such a simulation represents 100 square meters, too large a region to accurately analyze the fingering process, which takes place at the scale of centimeters to meters, depending on the properties of the aquifer.

The INCITE grant under which Lichtner and his team have conducted this carbon sequestration research also encompasses environmental remediation research using PFLOTRAN. By performing simultaneous multiple simulations for these remediation runs, PFLOTRAN has scaled up to 40,000 cores on Jaguar.

Lichtner noted that his team is working both to improve the performance of PFLOTRAN and to prepare for the arrival of even more powerful supercomputers. To make PFLOTRAN more effective, for example, the team is seeking to evolve from the use of a structured grid, in which a quarter of the cells are wasted to highly resolve regions of interest, to unstructured grids and adaptive mesh refinement that can place cells only where additional resolution is required.

Beyond that, he said, the team is anticipating a new generation of supercomputers capable of a million trillion calculations per second—an exaflop. At that scale Lichtner's team will be able to continue enhancing the PFLOTRAN code and refining simulations of the behavior of underground flow processes.

Contributors/Authors

Peter C. Lichtner, LANL

Principal Collaborators

Lichtner works with G. Bisht, J. Kumar, R. Mills, and B. Philip, ORNL; G.E. Hammond, PNNL; C. Lu, INL; B. Smith, Argonne; and D. Svyatskiy and A. Valocchi, University of Illinois–Urbana-Champaign.

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DOE, Scientific Discovery through Advanced Computing program, SciDAC-2, Groundwater Project

Publications

M. Person et al. 2010. "Assessment of Basin-Scale Hydrologic Impacts of CO_2 Sequestration, Illinois Basin." *International Journal of Greenhouse Gas Control* 4, no. 5: 840–854.

G.E. Hammond and P.C. Lichtner. 2010. "Field-Scale Model for the Natural Attenuation of Uranium at the Hanford 300 Area Using High-Performance Computing." *Water Resources Research* 46, no. 9: W09527. doi:10.1029/2009WR008819.

C. Lu et al. 2009. "Effects of Density and Mutual Solubility of a CO_2-Brine System on CO_2 Storage in Geological Formations: 'Warm' vs. 'Cold' Formations." *Advances in Water Resources* 32: 1685–1702.

C. Lu and P.C. Lichtner. 2007. "High Resolution Numerical Investigation on the Effect of Convective Instability on Long Term CO_2 Storage in Saline Aquifers." *Journal of Physics Conference Series* 78: 012042. doi:10.1088/1742-6596/78/1/012042.

Scientists Use Standard Candles to Illuminate Knowledge of the Universe

ABSTRACT

Type Ia supernovas, among the brightest exploding stars in the universe, are "cosmic yardsticks" whose application led to the discovery of dark energy. Astrophysicists are creating leadership computing simulations to better understand these explosions and by doing so help observers use them to determine the properties of dark energy.

Leadership-class computing provides an unparalleled ability to model and simulate Type Ia (thermonuclear-powered) supernovas. The ability to do 3D, large-scale simulations of these explosions led to the discovery of an entirely new and unexpected explosion mechanism, termed the gravitationally confined detonation (GCD) model, by researchers at the Flash Center for Computational Science at the University of Chicago.

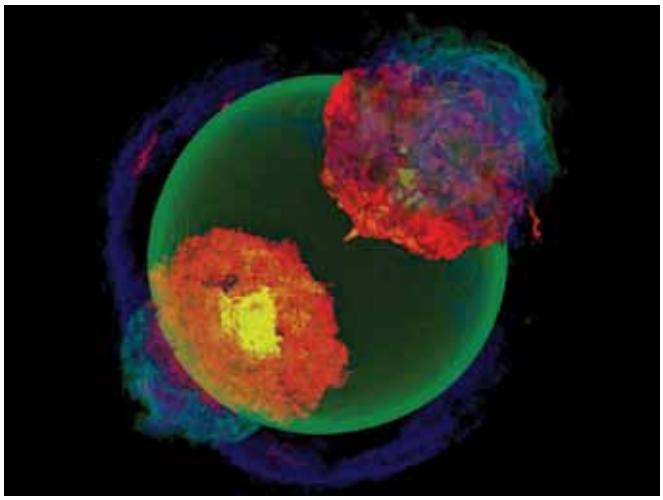
"This discovery illustrates the importance of being able to do 3D, whole-star simulations of these events and exemplifies scientific discovery through advanced computing," said Don Lamb, the center's director and the Robert A. Millikan Distinguished Service Professor in astronomy and astrophysics at the University of Chicago.

Lamb and his team at the Flash Center have done extensive simulations of Type Ia supernovas, as well as key physical processes important to the explosions, with computing time at DOE's ALCF awarded through the INCITE program. These events are thought to be white dwarf stars in binary systems that explode as a result of a runaway thermonuclear reaction. Type Ia supernovas are among the brightest explosions in the universe, making them important tools for measuring cosmological distances.

Observations using Type Ia supernovas as such cosmic yardsticks revealed that the expansion rate of the universe is accelerating and led to the discovery of dark energy, a hypothetical form of energy that permeates all of space. Understanding dark energy ranks among the most compelling problems in all of physical science.

The goal of the center's Type Ia supernova project is to better understand these explosions and by doing so help observers use them to determine the properties of dark energy. Improved understanding of dark energy has also been set as a 20-year priority by DOE.

Lamb and his team are using the FLASH computer code and the ALCF's IBM Blue Gene/P supercomputer, Intrepid, to conduct the first comprehensive, systematic validation of all current Type Ia models. As an important first step, the team has



Shown is a 3D, whole-star simulation of the GCD model of a Type Ia supernova at the moment at which a detonation wave begins to sweep through the white dwarf star, incinerating it. Image courtesy Flash Center for Computational Science, University of Chicago

conducted extensive simulations of buoyancy-driven turbulent nuclear combustion—a physical process that is key to Type Ia supernovas but not fully understood. The goal of the simulations is to provide definite answers to three questions:

1. Is it possible to describe the burning rate of a turbulent flame by a single characteristic turbulent timescale (or length scale)? If so, what is that scale?

2. Under what physical conditions does a flame transition from the flamelet regime to the distributed burning regime?

3. How does buoyancy-driven turbulent nuclear combustion differ from nuclear combustion in a homogeneous isotropic turbulent background?

Answers to these questions are needed in order to accurately model the nuclear flame in whole-star simulations of Type Ia supernovas and determine the physical conditions under which the flame is torn apart and transitions to distributed burning, a condition necessary for a deflagration-to-detonation transition as posited in one of the current Type Ia supernova models.

To address these questions, the team has done simulations for three physical settings: an initially planar flame in a column in which the density and acceleration of gravity are constant; an initially spherical flame bubble in an open domain in which the density and acceleration of gravity are constant; and an initially spherical flame bubble in a white dwarf star in which the density and acceleration of gravity strongly vary. The behavior of the flame is different in the three physical settings, enabling the

team to separate the effects of changes in density and gravitational acceleration on the properties of the flame.

The simulations show that the flame surface is complex at large scales and smooth at small scales and suggest that the so-called flame polishing length is the only length scale on which the burning rate depends. They also indicate that the transition to distributed burning occurs at a much smaller flame speed in the case of buoyancy-driven turbulent nuclear combustion than in that of nuclear combustion in the presence of fully developed turbulence. Finally, they reveal that the nuclear burning rate is smaller than it would be if the turbulence was fully developed. The Flash Center team is using this information to develop a better flame model for simulating Type Ia supernovas.

> This discovery illustrates the importance of being able to do 3D, whole-star simulations of these events and exemplifies scientific discovery through advanced computing.—Don Lamb, Flash Center for Computational Science, University of Chicago

The simulations of buoyancy-driven turbulent nuclear combustion and Type Ia supernova explosions are huge, with some runs consuming all 160,000 processors of Intrepid. A checkpoint file (which contains all the information needed to restart the simulation from that point in time) can be hundreds of gigabytes in size, and the data produced by a single simulation can total tens of terabytes.

Such enormous amounts of data require leadership-class storage resources. In collaboration with Argonne's Mathematics and Computer Science Division, researchers use a technique called parallel I/O to write out the data produced by Intrepid's processors. To provide high data transfer rates, Intrepid's storage system contains more than 9,000 disk drives connected through 128 storage servers. Parallel I/O libraries manage all those disks and server connections to reduce the time needed to transfer data, allowing more time for computational science.

The Flash Center team's 3D, whole-star simulations of Type Ia supernovas have produced new insights into how these stars explode. They have also led to the discovery of robust signatures for the different supernova models, holding the promise that observations can discriminate among them.

Now the center's team is working with the Sloan Digital Sky Survey II (SDSS-II) Supernova Survey Team and its collaborators to confront the light curves and spectra predicted by the simulations with high-quality data. Preliminary results show that the light curves predicted by the GCD model can be fit reasonably well by the data-driven models the supernova community uses to fit the light curves of individual Type Ia supernova, demonstrating that the predicted light curves are similar to those observed. Preliminary results based on 2D simulations show the light curves predicted by the GCD model are consistent with the observed relation between peak luminosity and rate of fading. The results also suggest that the anomalous scatter in the calibration of these supernovas as cosmic yardsticks may be due in part to the difference in how the intrinsically asymmetric supernovas look when viewed from various directions.

Contributors/Authors

Don Q. Lamb, Anshu Dubey, Sean Couch, Christopher Daley, Benedict Diemer, Robert Fisher, Norbert Focke, Jonathan Gallagher, Carlo Graziani, Randy Hudson, George Jordan, Rick Kessler, Yeunjin Kim, Min Long, John Norris, Michael E. Papka, Katherine Riley, Daan van Rossum, Dean Townsley, and Klaus Weide, Flash Center for Computational Science, University of Chicago.

Principal Collaborators

The contributors work with the Sloan Digital Sky Survey II Supernova Survey Team: Joshua Frieman (Fermilab and Department of Astronomy and Astrophysics, University of Chicago); and Dan Kasen (LBNL and Department of Astronomy, University of California–Berkeley).

Funding

DOE NNSA Advanced Simulation and Computing Academic Strategic Alliance Program under contract to the Center for Astrophysical Thermonuclear Flashes at the University of Chicago; NNSA Advanced Simulation and Computing Program; DOE Office of Science, ASCR; DOE through the Argonne Institute for Computing in Science under contract to Argonne; and NSF Astronomy and Astrophysics Program.

Publications

D. M. Townsley et al. 2007. "Flame Evolution during Type Ia Supernovae and the Deflagration Phase in the Gravitationally Confined Detonation Scenario." *The Astrophysical Journal* 668: 1118–1131.

G. C. Jordan IV et al. 2008. "Three-Dimensional Simulations of the Deflagration Phase of the Gravitationally Confined Detonation Model of Type Ia Supernovae." *The Astrophysical Journal* 681: 1448–1457.

C.A. Meakin et al. 2009. "Study of the Detonation Phase in the Gravitationally Confined Detonation Model of Type Ia Supernovae." *The Astrophysical Journal* 693: 1188–1208.

R. Bair et al. In press. "Verification and Validation of Current Models of Thermonuclear-Powered Supernovae Using Large-Scale Simulations." *Journal of Physics: Conference Series* (London: IOP Publishing).

Researchers Break Petaflop Barrier with Study of Electrons in Computer Chips

ABSTRACT

A team that models electrons traveling through transistors ran a scientific application at more than a thousand trillion calculations per second. The application may accelerate the development of semiconductors through which electrons can zip with less resistance, using less energy and generating less heat than in traditional devices.

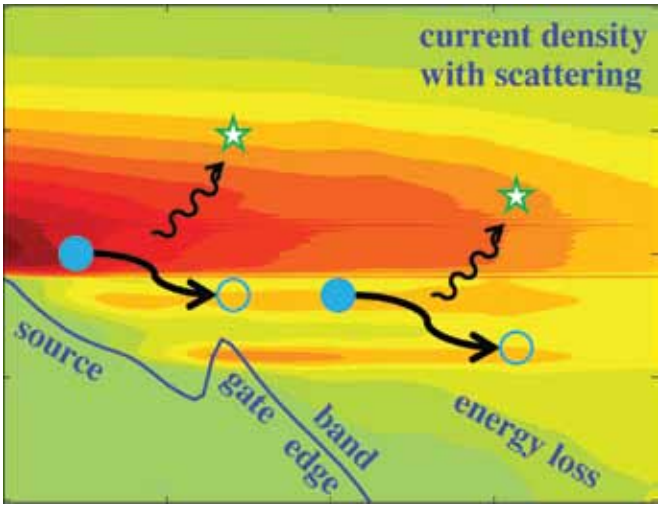
Researchers at Purdue University used ORNL's Jaguar supercomputer to model the journey of electrons as they travel through electronic devices. Gerhard Klimeck, leader of Purdue's Nanoelectronic Modeling Group, and Mathieu Luisier, a member of the university's research faculty, used more than 220,000 of Jaguar's 224,000 processing cores to reach 1.03 petaflops with OMEN, one of only five scientific application codes ever to break the petascale barrier (all of which have run on Jaguar).

"We build models that try to represent how electrons move through transistor structures," Klimeck explained. "The goal is to design new nanometer-scale devices with novel materials and geometries to reduce the energy that is consumed during the switching operations, make the devices smaller, and yet make them run faster."

The work closely aligns with a DOE 20-year priority to study nanoscale science for new materials and processes. The team aims to help manufacturers transcend Moore's Law, which since 1965 has anticipated the astonishing pace of technological advances. In that year Intel cofounder Gordon Moore suggested in *Electronics* magazine that the density of transistors on a computer chip—and therefore the speed of that chip—would double about every 2 years. And indeed they have, with Moore's company in 2011 releasing chips that hold more than 2 billion transistors on a piece of silicon just over an inch square.

But there is a limit to how many transistors will fit onto a silicon chip. Within the next few years, transistors will be as small as they can get. "We're at the stage where these transistors—the on-off switches—in these chips are as small as 20 to 30 nanometers in some of their critical widths," noted Klimeck. "That's along the lines of 100 to 150 atoms. We're beginning to reach a limit where making it another factor of two smaller is going to be more and more difficult."

Jaguar's power has allowed Klimeck and Luisier to pursue this task with unprecedented realism. "You're reaching the stage where you can't think of your material being like a continuum," Klimeck said. "We experience that this material is not continuous but discrete. The placement of these atoms is important."



In a nanowire, electrons (filled blue circles) lose energy by emitting phonons, or crystal vibrations (green stars), as they move from the source to the drain and pass through the gate of the transistor. Image courtesy Gerhard Klimeck and Mathieu Luisier, Purdue University

The team is pursuing this work with two applications, known as Nanoelectric Modeling (NEMO) 3D and OMEN (a more recent effort). NEMO 3D is an evolution of the earlier NEMO 1D, developed at Texas Instruments in the mid-1990s to model resonant tunneling diodes—devices that used the QM ability of electrons to tunnel through a tiny barrier and appear on the other side. NEMO 3D expanded the application to three dimensions and million-atom systems, but at a cost: The code could model only static systems (that is, with no electron flow).

"We were able to say where the electrons would be sitting in this geometry, but we couldn't afford computationally to model electrons injected at one end and pulled out at the other end, which we did do in NEMO 1D but in a one-dimensional space or representation," Klimeck said.

"Around 2004 compute powers became strong enough on massively parallel machines that we could dream of combining the NEMO 1D and NEMO 3D capabilities and represent the device in three dimensions one atom at a time and inject electrons at one end and pull them out at the other end. OMEN was born," he said. "Having machines like Jaguar made these calculations possible. The theory of how to atomistically represent a device in 3D and follow the flow of electrons through it was understood with NEMO 1D, but it was computationally prohibitively expensive. The next-generation code, OMEN, now makes it feasible to run on Jaguar."

These applications calculate the behavior of the most important quantum particles in the system—valence electrons, which are located in atoms' outermost shells—from their fundamental

properties. These are the electrons that flow freely in the device and produce current. In contrast, the applications approximate the behavior of other particles—the atomic nuclei and electrons on the inner shells. The applications solve the Schrödinger equation, which describes the QM properties of a system. Luisier has modified the simulation's boundary conditions to allow for electrons moving into and out of the system. Using OMEN he has been able to model about 140,000 atoms. Without taking into account the flow of electrons, NEMO 3D can simulate 5 million to 10 million atoms.

> The theory of how to atomistically represent a device in 3D and follow the flow of electrons through it was understood with NEMO 1D, but it was computationally prohibitively expensive. The next-generation code, OMEN, now makes it feasible to run on Jaguar.—Gerhard Klimeck, Purdue University

At this scale the QM oddities of electrons, such as the tunneling behavior studied in NEMO 1D, become increasingly important. "Our understanding of electron flow in these structures is different," Klimeck explained. "As you make things very small, you expose the quantum mechanical nature of the electrons. They can go around corners. They can tunnel. They can do all kinds of crazy stuff."

Insights to improve electronic devices

The team is working with two experimental groups to improve practical devices. One is led by Jesus Del Alamo at the Massachusetts Institute of Technology, the other by Alan Seabaugh at Notre Dame.

With Del Alamo's group the team is looking at making the electrons move through a semiconductor faster by building it from indium arsenide rather than silicon.

"If electrons move faster in nanoscale transistors, they will in general lose less energy and can be controlled more rapidly, resulting in lower resistance and higher switching speeds," Klimeck noted.

With Seabaugh's group the modeling team is working on band-to-band-tunneling transistors. These transistors bear some promise in lower-voltage operation as they have different thermal carrier distributions compared to standard silicon transistors.

As the transistor dimensions shrink, more devices are packed closer together, consuming relatively more power in the same area. The power consumption reflects itself in local heating, which now needs to be critically understood.

"Atoms like to vibrate in certain ways, and the vibrations are losses that come out of the device as heat," Klimeck said. "If we understand how the electrons interact with the semiconductor crystal at the nanometer scale, how heat is being generated, maybe we can avoid the heat and make the transistors less power hungry. On the flip side we may be able to improve devices that convert thermal energy into electricity."

Minimizing the power requirements and heat generation of electronics as well as harvesting energy are critically important as our lives become more and more automated.

"This is important anyplace where you don't want to lug 40 pounds of batteries with you, for instance, if you'd like your iPhone to be lighter and run all kinds of image processing on it," Klimeck noted. "This is true for any mobile or computing technology—anything where you don't want to waste energy, which these days is anywhere."

Contributors/Authors

Gerhard Klimeck and Mathieu Luisier, Purdue University

Principal Collaborators

Jesus Del Alamo at the Massachusetts Institute of Technology builds semiconductors from indium arsenide. Alan Seabaugh at Notre Dame works on band-to-band-tunneling transistors.

Funding

DOE Office of Science, Army Research Office, Midwest Institute for Nanoelectronics Discovery, NSF, and Sandia

Publications

M. Luisier and G. Klimeck. 2009. "Atomistic Full-Band Simulations of Silicon Nanowire Transistors: Effects of Electron-Phonon Scattering," *Physical Review B* 80: 125202.

M. Luisier and G. Klimeck. 2010. "Simulations of Nanowire Tunneling Transistors: From the WKB Approximation to Full-Band Phonon-Assisted Tunneling," *Journal of Applied Physics* 107: 084507.

M. Luisier and G. Klimeck. 2010. "Phonon-Limited Mobility and Injection Velocity in n- and p-Doped Ultrascaled Nanowire Field-Effect Transistors with Different Crystal Orientations," *Proceeding of the International Electron Device Meeting (IEDM 2010), San Francisco CA, USA*, December.

M. Luisier. 2010. "A Parallel Implementation of Electron-Phonon Scattering in Nanoelectronic Devices Up to 95K Cores," *Proceeding of the Supercomputing Conference SC10, New Orleans, LA*, November.

Computation Proves Predictive Capabilities of Nuclei through Fluorine-14 Simulation

ABSTRACT

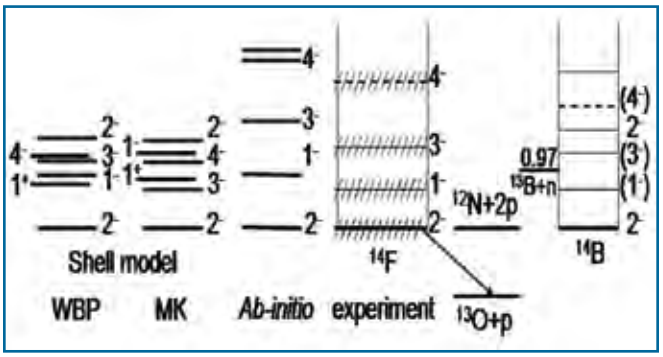
Using the Argonne and Oak Ridge Leadership Computing Facilities' supercomputers, researchers are comprehensively defining stable and unstable nuclei, essential in fusion and fission energy. Accurate simulations of fluorine-14, recently corroborated by experiment, help scientists gain insight into the behavior of nuclei never before measurable.

Fluorine-14 is a very unstable isotope; it typically lives far less than a microsecond before releasing a proton and becoming the more stable oxygen-13. Short-lived nuclei are bountiful in both natural and man-made settings, but until recently, their short life spans have prevented scientific researchers from learning about their natures. By refining simulations over time, one team hopes to predict the properties of nuclei in fission and fusion reactors, gaining insight into how to make these power sources commercially viable.

As part of its quest to understand fluorine-14, a team led by Iowa State University physicist James Vary used ALCF and OLCF resources to predict the behavior of this relatively unknown isotope. It published its predictions in *Physical Review C* in February 2010. Six months later a group of researchers at Texas A&M University's Cyclotron Institute performed an experiment producing fluorine-14, and the results nearly mirrored those of Vary's group.

"Simulations have come to the stage of development where they are so precise that they can actually predict with some accuracy experimental results that have not yet been obtained," Vary said. The team used the ALCF's IBM Blue Gene/P, Intrepid, and the OLCF's Cray XT5, Jaguar, supercomputers to run the Many Fermion Dynamics-nuclear (referred to as MFDn) code for an ab initio simulation of fluorine-14, meaning simulations focused on careful treatment of the neutron–neutron, neutron–proton, and proton–proton interactions responsible for predicted states of the element. The largest simulations ran on about 30,000 of the Jaguar's 224,256 processing cores, and the team ran many simulations before submitting its predictions. "We held our breath," Vary said in reference to waiting for experimental data to come from the Cyclotron Institute.

The research fits well with DOE's mission to explore extreme forms of nuclear matter, an area in which man has limited understanding despite the fact that nuclei make up 99 percent of visible matter. By charting the behavior of fluorine-14, the team's research lays the groundwork for observing the strong interactions of subatomic particles in other unstable isotopes, moving toward a clear and comprehensive image of this type of nuclear matter and its properties. These comprehensive definitions take science closer to experimentally defining more unstable isotopes at DOE's Facility for Rare Isotope Beams.



The Vary team made predictions on the behavior of fluoride-14 and published its results in *Physical Review C*. The team's predictions (ab initio bars) nearly matched an experiment done 6 months later at Texas A&M's Cyclotron Institute (experiment bars). Image courtesy Texas A&M University Cyclotron Institute

The Vary team is supported by ALCF and OLCF resources through the INCITE program and NERSC resources. It is funded through multiple awards under the Scientific Discovery through Advanced Computing program, ASCR, and DOE grants. It is also part of a larger project aiming to define properties of all isotopes, Universal Nuclear Energy Density Functional (or UNEDF, for short), in which researcher Steven C. Pieper is working under the same INCITE allocation using 32,768 cores on the IBM Blue Gene system at Argonne to make calculations of states of the carbon-12 nucleus.

Intricate interactions

In addition to predicting the mass and low-lying, excited-state behavior of the fluorine-14 nucleus, Vary's team also correctly predicted that these unstable isotopes would stabilize by decaying proton emission, or "proton dripping," which results in a lighter nuclei. "We can think of it as a wet sponge," Vary said. "Fluorine-14 has protons in it, but it can't hold them, so it must let one out very quickly. It doesn't come out with a lot of energy but enough to be observed."

Many unstable nuclei appear for only microseconds and in many cases only in situations that would be very difficult to observe experimentally. Nuclear power reactors, for instance, create many short-lived materials during a nuclear reaction capable of influencing energy generation in reactors. "You can produce something that only lives for a second or two, but during that time it can absorb additional neutrons in the reactors," Vary said.

Vary pointed to three main issues that make the project computationally difficult. The quantum many-particle problem means that the simulation must not only account for large numbers of particles interacting with one another but also for the quantum mechanics—in which subatomic particles exhibit both particle-like and wave-like characteristics—that must be calculated with high accuracy.

The second issue comes from the extremely strong interactions among the neutrons and protons. Vary said that many of the conventional tools physicists use to study particles are not applicable to their simulations of unstable nuclei. "We want to make sure we don't lose some of the inherent predictive power that comes with treating [strong interactions] carefully," Vary said. By treating both the quantum and strong interactions with such precision, a third issue arises in the massive calculations that must be performed to generate meaningful data for comparison with experiments.

> Simulations have come to the stage of development where they are so precise that they can actually predict with some accuracy experimental results that have not yet been obtained.—James Vary, Iowa State University

ORNL's David Dean was principal investigator on the first 3-year INCITE project, which ran from 2008 to 2010. The team secured another 3-year allocation beginning in 2011 to work toward the same goals, and Vary, this project's principal investigator, said he and his partners are definitely looking forward to continued collaboration with leadership computing facilities. "We're very excited about the convergence of the technical capabilities that these new facilities represent with our own theoretical and algorithmic capabilities, meaning that we can productively use these new tools," Vary said.

Contributors/Authors

James Vary, Iowa State University

Principal Collaborators

Principal scientific collaborators are Steven Pieper of Argonne, Pieter Maris of Iowa State University, Joseph Carlson and Petr Navratil of LLNL, Andrey Shirokov of Moscow State University, Hai Ah Nam and David Dean of ORNL, and Witold Nazarewicz of University of Tennessee–Knoxville.

Funding

DOE Office of Science, Nuclear Physics Program and ASCR; DOE NNSA; NSF PetaApps Program; and ORNL, Argonne, LLNL, and LANL

Publications

J.P. Vary et al. 2009. "*Ab Initio* Nuclear Structure—the Large Sparse Matrix Eigenvalue Problem." *Journal of Physics: Conference Series* 180: 012083.

P. Maris, A. M. Shirokov, and J.P. Vary. 2010. "*Ab Initio* No-Core Full Configuration Calculations of Light Nuclei." *Physical Review C* 81 (February 4): 024315.

P. Maris et al. 2010. "Scaling of *Ab-Initio* Nuclear Physics Calculations on Multicore Computer Architectures." *Procedia Computer Science* 1: 97–106.

V.Z. Goldberg et al. 2010. "Proton-Dripping Fluorine-14." *Physical Review Letters B* 692: 307.

Computing Yields Insights on Ways to Reduce Energy Dissipation in Transportation

ABSTRACT

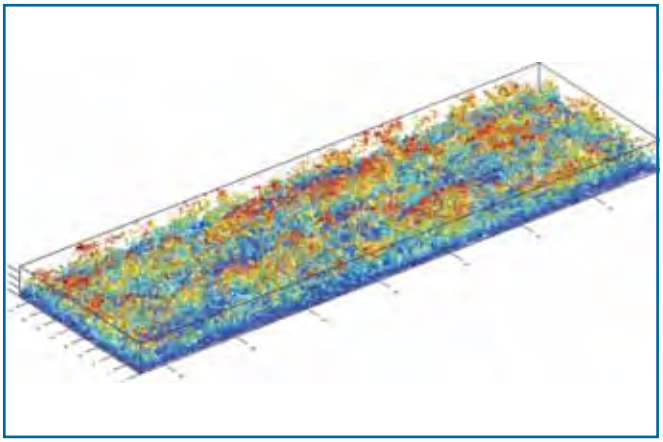
Simulations using an Argonne Leadership Computing Facility supercomputer assist researchers in probing the physics of turbulent flow phenomena. Taking a new scientific approach, researchers now have a better understanding of boundary layers—the primary interfaces between a vehicle and the medium in which it moves—and that new knowledge may lead to more energy-efficient vehicle design.

Transportation accounts for approximately 28 percent of energy consumption in the United States. Central to energy losses inherent in transportation is turbulence at the boundary layer between a vehicle and the medium through which it moves. The energy expenditure results from the interaction between the solid surfaces of vehicles or pipes and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. This drag is caused by friction and pressure at the vehicle's surface that are enhanced when the boundary layers peel off, slowing the vehicle and consuming energy.

Currently a lack of accurate models of turbulence phenomena impedes engineering developments to reduce this drag and corresponding energy consumption. By performing DNSs of turbulent flow exerting strong inertial and viscous forces in a boundary layer, however, researchers from the University of Texas–Austin and Universidad Politécnica de Madrid led by Robert Moser and Javier Jimenez are gaining insights to aid creation of such models and new concepts to manipulate the boundary layers for improved vehicle design. Their work aligns with DOE's mission to provide solutions to the nation's energy challenges.

"Simulations on the most advanced supercomputers enable turbulence research by exposing the structure of turbulence in unprecedented detail," said Moser. "Supercomputer simulations of turbulence like those conducted at the ALCF are a game changer for scientists. With them progress is not limited by what can be measured, only by the insight of the investigator."

A key issue in DNS, which computes turbulent eddies at their smallest and largest scales, is the Reynolds number, a measure of the relative importance of inertia and viscosity. Larger Reynolds numbers imply stronger inertia. Moreover, the larger the Reynolds number, the greater the resolution requirements (and cost) of DNS—and generally the greater the relevance to technological applications. When performing DNSs the researchers are interested in scaling the simulation results to much larger Reynolds numbers, which requires that the Reynolds numbers simulated be sufficiently large to expose the behavior in such regimes.



A visualization of the velocity in a boundary layer at Reynolds numbers up to 2100 shows the growth of the turbulence structures out into the free stream as it evolves downstream (to the right) and the intermittent uneven boundary of the turbulent region. Image courtesy Juan Sillero, Universidad Politécnica de Madrid

The researchers' goal is to address the poor understanding of the zero-pressure-gradient (ZPG) turbulent boundary layer (the layer of fluid next to a surface, usually a solid) on a flat plate, which serves as the prototype for turbulent boundary layers, such as those on vehicles. Even for this long-studied, simple case, there is much less information available than for internal flows (such as the flow of fluids through pipes) and many questions remain. An important problem has been the difficulty of experimentally measuring the stress along the boundary wall, which makes scaling results ambiguous. Furthermore, the turbulence in internal flows dissipates differently from jets into air, and it has also proven difficult to measure its behavior.

"Direct numerical simulations remove most of those difficulties," noted Moser. "Not only can 'everything' be measured, but the equations of motion are also directly accessible, allowing the different processes to be evaluated and quantified."

New approach leads to insights

One challenge to performing DNS of a boundary layer at a high Reynolds number comes from streamwise development. While simple internal turbulent flows such as those through pipes are uniform in the streamwise direction, boundary layers develop continuously. Using the ALCF's IBM Blue Gene/P system, Moser and his team developed a new approach to effectively simulate a longer spatial domain by breaking the domain into two shorter pieces. A flat surface at the end of the first domain serves as an inlet condition for the second. This innovation has a significant advantage over past approaches because the first domain can be simulated with much coarser resolution, making it about ten times less expensive to simulate this portion than it would be to do so if it were part of a unified single simulation. This

approach has been implemented and tested using 34 million processor hours—including 29 million processor hours that used more than 20 percent of the machine—and typically 32,768 cores for each job. Coarse-resolution simulations based on the new approach are now being calculated to eliminate statistical transients.

Simulations on the most advanced supercomputers enable turbulence research by exposing the structure of turbulence in unprecedented detail. Supercomputer simulations of turbulence like those conducted at the ALCF are a game changer for scientists. With them progress is not limited by what can be measured, only by the insight of the investigator.—Robert Moser, University of Texas–Austin

As a result of its simulations, the research team discovered that at large Reynolds numbers, the boundary layer slowly relaxes from the artifacts of the inlet conditions. This behavior appears to be physical (that is, not an artifact of the computation) and implies that boundary layers have longer "memories" than previously thought, meaning the effects of any disruption or purposeful manipulation will persist for longer downstream. This is good news if one is trying to engineer the evolution of the boundary layer, though it proved inconvenient for the researchers simulating a standard boundary layer.

In the near future, simulations of these high-Reynolds-number boundary layers will be completed. The hard work of analyzing the simulation results to uncover the inner workings of this important turbulent flow will then begin. Researchers will in effect conduct computer experiments whereby measurements to expose the characteristics of the turbulence are made computationally using the data stored from the simulations.

Contributors/Authors

Robert Moser, University of Texas–Austin and Javier Jimenez, Universidad Politécnica de Madrid

Principal Collaborators

Principal scientific collaborators are Javier Jimenez of Universidad Politécnica de Madrid, who is leading the boundary layer analysis effort; Juan Sillero of Universidad Politécnica de Madrid, who is developing the simulation code and executing the simulations; and Nicholas Malaya, who is acting as a consultant for software engineering and compute and I/O performance.

Funding

DOE Office of Science, ASCR; DOE NNSA; and NSF, Office of Cyberinfrastructure. NNSA's contribution is through the Predictive Science Academic Alliance Program (the Center for Predictive Engineering and Computational Sciences at the University of Texas). The organization's interest in this context is in reliable turbulence data for validation and uncertainty quantification.

Publications

J. Jimenez et al. 2008. "Turbulent Fluctuations Above the Buffer Layer of Wall-Bounded Flows." *Journal of Fluid Mechanics* 611 (August 26): 215–236.

J. Jimenez et al. 2007. "What Are We Learning from Simulating Wall Turbulence?" *Philosophical Transactions of The Royal Society* A 365, no.1852 (March 15): 715–732.

S. Hoyas et al. 2006. "Scaling of the Velocity Fluctuations in Turbulent Channels Up to Re=2003." *Physics of Fluids* 18: 011702.

M. P. Simens et al. 2009. "A High-Resolution Code for Turbulent Boundary Layers." *Journal of Computational Physics* 228, no. 11 (June 20): 4218–4231.

Leadership Computing Shows Dark Matter Clumped to Birth Galaxies

ABSTRACT

Using the Oak Ridge Leadership Computing Facility's Jaguar supercomputer, researchers charted dark matter through the universe's development over billions of years. The simulation was the largest of its type at the time and moved humanity one step closer to understanding how our universe got to its current state.

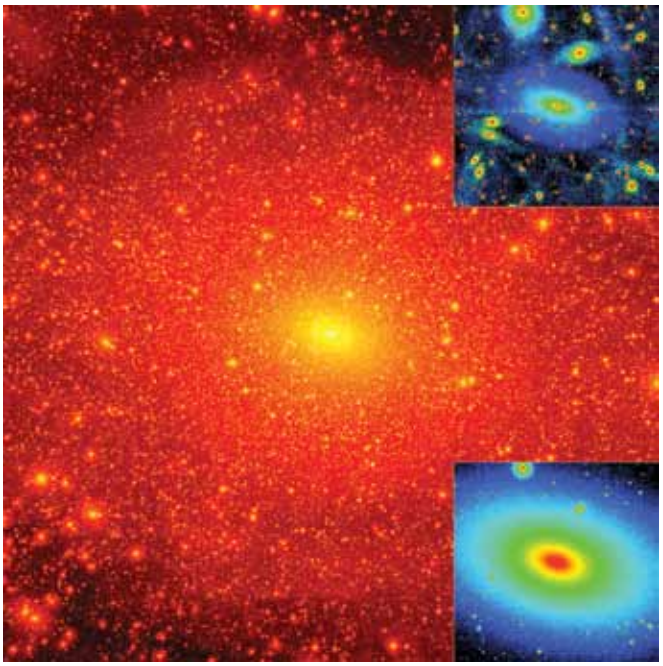
Armed with a knowledge of how gravity works and extensive observations, scientists have concluded that less than one-fifth of the matter in the universe is visible. Researchers have observed the motion of gas and stars within galaxies, galaxies within clusters, and the cosmic microwave background, and the remainder—dark matter—has no interaction with regular matter except through the force of gravity. Nevertheless, dark matter provides the invisible scaffolding surrounding the sites in which luminous galaxies and stars actually form.

A team led by astrophysicist Piero Madau of the University of California–Santa Cruz used Jaguar to run what was at that time the largest simulation of dark matter evolving over billions of years to envelop a galaxy such as our own Milky Way. The simulation followed a galaxy's worth of dark matter through nearly the entire history of the universe, dividing the dark matter into more than a billion separate parcels, each 4,000 times as massive as the sun. It was a staggering job that involved tracking 9×10^{21} tons of invisible stuff spread across 1.76×10^{20} square miles as it evolved over 14 billion years.

The project attempting to illuminate dark matter was given an allocation of supercomputer time through the INCITE program. It used about 1.5 million processor hours on the Jaguar HPC system located at the OLCF at ORNL. The work aligns with a DOE goal to clarify the origins of matter.

"The simulation showed for the first time the fractal-like appearance of dark matter substructures," Madau said. "It suggests that at infinite resolution one would find a long, nested series of dark matter clumps within clumps within clumps, reminiscent of a Russian Matryoshka doll, all the way down to the first and smallest Earth-mass dark matter lumps that formed in the early universe."

Using initial conditions provided by observations of the cosmic microwave background, Madau and his team were able to simulate dark matter through a computer application called PKDGRAV2. "The computer was basically just computing gravity," Madau explained. "You have to compute the gravitational force between 1 billion particles, and to do that is very tricky.



The Madau team's "Via Lactea II" simulation was the largest of its type to date. Each pixel simulated a mass 4,100 times that of our sun and about 760 trillion miles wide. The inset images focus on phase-space (top) and local (bottom) densities on an inner cube of the simulation. Image courtesy Piero Madau

You're following the orbits of these particles in a gravitational potential that is varying all the time. The code allows you to compute with very high precision the gravitational force due to the particles that are next to you and with less and less precision the gravitational force due to the particles that are very far away because gravity becomes weaker and weaker with distance." PKDGRAV2 is what is called a hierarchical tree code, which makes gigantic calculations tractable because it reduces the number of operations necessary to compute the gravitational interactions between N particles from N^3 to N^2.

Dark matter is not evenly spread out, although researchers believe it was nearly homogeneously distributed right after the Big Bang. Over time, however, it became bunched and clumped as gravity pulled it together, first into tiny clumps more or less the mass of the Earth. These clumps were pulled together into larger clumps, which were pulled together into still larger clumps, and so on until they combined to form halos of dark matter massive enough to host galaxies. One key question has been whether smaller clumps would remain identifiable or smooth out within larger galactic halos. Madau's simulation provided enough resolution to verify that subclumps and sub-subclumps do indeed survive, even in the very inner regions in which our solar system is located.

Madau's team will verify its simulation results using NASA's Fermi Gamma-Ray Space Telescope (formerly GLAST), launched in 2008 to study extreme and puzzling phenomena: gamma-ray bursts, neutron stars, supernovas, and dark matter. Researchers believe that dark matter particles and antiparticles may annihilate each other when they collide, producing gamma rays that can be observed from space. The clumpiness that Madau's simulations predict should increase the likelihood of dark matter particles encountering one another, and therefore should produce copious gamma rays. The team produced artificial observations of this enhanced gamma-ray production that can be directly compared to GLAST observations. A second verification comes from gravitational lensing, in which the gravity that a galaxy exerts along the line of sight bends the light traveling from faraway quasars. If the dark matter halos of galaxies are as clumpy as this simulation suggests, the light from a distant quasar should be lensed. "We already have some data there," Madau noted. "Our simulation seems to produce the right amount of lumpiness." The detection of gamma-ray annihilation from dark matter clumps in the halo of the Milky Way is one of the most exciting discoveries that the orbiting Fermi satellite could make, confirming the quantitative predictions of Madau and collaborators.

> The simulation showed for the first time the fractal-like appearance of dark matter substructures.—Piero Madau, University of California–Santa Cruz

Although simulations made predictions for what might be observed in the future, other results of the simulations seem to contradict current observations. For example, Madau noted that while dark matter in the galaxy is very clumpy, that same feature is not found in visible matter. In fact, far fewer dwarf galaxies orbit the Milky Way than simulation might predict.

"We see as many as 20 dwarf galaxy satellites of the Milky Way that are luminous," he explained, "and we estimate that there may be a hundred or so. But we predict thousands of relatively massive dark matter clumps. So there seems to be a conflict between the relatively smooth stellar halo of the Milky Way and the extremely clumpy dark matter distribution. Clearly stars are not forming in most of the dark matter lumps that we find in the simulation. Understanding this 'missing satellite problem' is key to developing a self-consistent theory of galaxy formation in the universe."

Contributors/Authors

Piero Madau, University of California–Santa Cruz

Principal Collaborators

Principal scientific collaborators are Michael Kuhlen of the University of California–Berkeley; Juerg Diemand, Ben Moore, Doug Potter, and Joachim Stadel of the University of Zurich; and Marcel Zemp of the University of Michigan.

Funding

NASA and NSF

Publications

M. Kuhlen et al. 2009. "Exploring Dark Matter with Milky Way Substructure." *Science* 325, no. 5943 (August 12): 970–973.

M. Zemp et al. 2009. "The Graininess of Dark Matter Haloes." *Monthly Notices of the Royal Astronomical Society* 394, no. 2 (March 4): 641–659.

J. Diemand et al. 2008. "Clumps and Streams in the Local Dark Matter Distribution." *Nature* 454, no. 7205 (August 7): 735–738, May 27.

M. Kuhlen et al. 2008. "The Dark Matter Annihilation Signal from Galactic Substructure: Predictions for GLAST." *The Astrophysical Journal* 686, no. 1 (October 10): 262–278.

Supercomputers Aid in Understanding the Basic Building Blocks of Nature

ABSTRACT

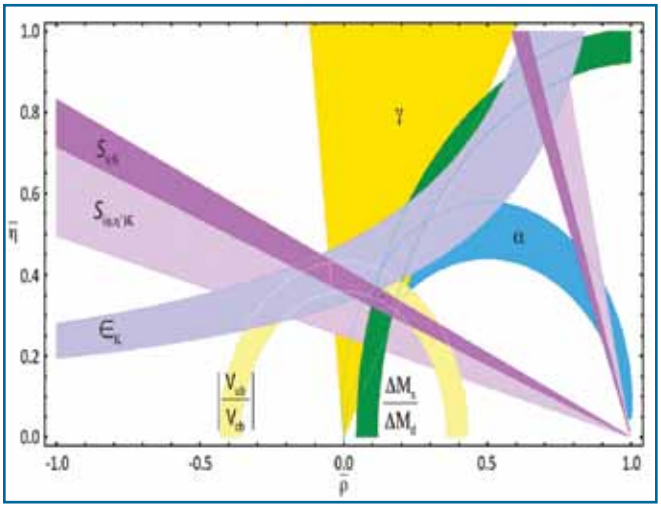
Using Oak Ridge and Argonne Leadership Computing Facility supercomputers, researchers are studying the interactions between quarks and gluons, two subatomic building blocks of matter. Their findings have led to significant advances in high-energy and nuclear physics. Their calculations have been essential in interpreting nuclear physics, heavy-ion collision, and high-energy experiments. More precise calculations will aid in the search for particles and forces not yet discovered.

Schoolchildren learn that atoms, the building blocks of matter, are composed of such particles as protons, neutrons, and electrons. Scientists know that protons and neutrons contain even smaller particles called quarks and gluons. Nearly all the visible matter in the universe is made up of these tiny subatomic particles. While the behavior of protons and neutrons is well understood, less is known about the interactions of quarks and gluons.

However, scientists do recognize that quarks and gluons interact in fascinating ways. For example, the force between two quarks increases as they move apart. Quarks are classified into six categories—up, down, charm, strange, bottom, and top—depending on their properties. Gluons, on the other hand, can capture energy from quarks and function as glue to bind quarks. Groups of gluons can also bind, forming glueballs. Scientists have identified another unique property of gluons, which they describe as color. Quarks can absorb and give off gluons, and when they do so, they are said to change color. It is also believed that quarks seek to maintain a state of color balance, and the process of absorbing and shedding gluons helps them achieve that balance.

The scientific community thinks the four fundamental forces of nature—electromagnetism, gravity, the strong force (which holds an atom's nucleus together), and the weak force (responsible for quarks' ability to change color)—are related. The study of the strong interaction in terms of quarks and gluons is called quantum chromodynamics, or QCD.

A team of scientists from seven institutions of higher learning, collaborating under the leadership of Paul Mackenzie of Fermi National Accelerator Laboratory, has been awarded a total of 80 million processor hours at the OLCF and the ALCF for QCD research to help develop a unified theory of how the four forces interact. Physicists believe that more fundamental interactions must exist that unite the presently observed forces. Supercomputing aids in the search for this new physics by making possible the comparison of current theories with experiment so anomalies can be sought.



Lattice QCD calculations of strongly interacting particles enable increasingly precise determinations of the parameters of particle physics. Image courtesy E. Lunghi of Indiana University, J. Laiho of the University of Glasgow, and R. Van de Water of Brookhaven National Laboratory

A four-dimensional lattice model

Because quarks and gluons interact differently than do protons and neutrons, researchers are employing a different methodology for their study. The continuous path elementary particles follow through space and time by hops on a four-dimensional lattice model is a process referred to as discretization. The team uses supercomputers to perform calculations to relate experimentally observed properties of these strongly interacting particles to QCD.

The highly advanced computational power of the Cray XT4/XT5 (at the OLCF) and IBM Blue Gene/P (at the ALCF) supercomputers enables the research team to produce and validate high-precision lattice QCD calculations that are essential to the analysis of recently completed experiments in high-energy and nuclear physics and other studies currently in progress. Simulations are used to relate the fundamental theoretical equations governing quarks and gluons to predictions of physical phenomena made in laboratories.

"Leadership-class computing makes it possible for researchers to generate such precise calculations that someday theoretical uncertainty may no longer limit scientists' understanding of high-energy and nuclear physics," said Mackenzie.

Using Monte Carlo techniques to predict the random motions of particles, the simulations generate a map of the locations of up, down, and strange quarks on a fine-grained lattice. The up and down quarks have masses sufficient to enable researchers to extrapolate physical properties.

Employing fundamentals from the Standard Model of subatomic physics, team members are exploring quark properties and dynamics. They are trying to determine the mass spectrum and coupling of strongly interacting particles and the electromagnetic properties of particles made up of interacting quarks (baryons and mesons) to create an understanding of a nucleon's internal structure.

The team is studying three distinct quark actions—clover, domain wall, and improved staggered—and validating calculations that cannot be checked through direct comparison with experiment by performing them with more than one method of discretizing the equations.

The researchers have completed domain-wall configuration ensembles of lattice spacings of 0.114 and 0.086 femtometers on lattices of sizes $24^3 \times 64$ and $32^3 \times 64$, respectively, where in expressions such as $24^3 \times 64$, 24 is the number of lattice sites in the 3 spatial directions and 64 is the extent of the lattice in time. These are the largest domain-wall lattices ever attempted and will allow calculations with smaller lattice spacings and therefore smaller discretization errors than ever before achieved with domain-wall fermions. For the staggered quarks, the team has completed a set of runs with lattice spacings of 0.06 and 0.045 femtometers. These are the largest, most computationally challenging staggered ensembles generated to date.

Leadership-class computing makes it possible for researchers to generate such precise calculations that someday theoretical uncertainty may no longer limit scientists' understanding of high-energy and nuclear physics.—Paul B. Mackenzie, Fermi National Accelerator Laboratory

These ensembles are currently being analyzed in studies of the decays and mixings of particles containing heavy quarks to enable major improvements in determining a number of elements in the quark mixing matrix. The calculations are enabling precise tests of the Standard Model, aiding in a deeper understanding of fundamental physics.

Improved versions are being created for both the domain-wall and staggered methods for formulating the continuum equations for fermions on a discrete lattice. A new method has been developed for domain-wall fermions (the Aux Det method), which will permit calculations with smaller quark masses. (Previous calculations were done with quark masses that were larger than those in real life because calculations with heavier quark masses require smaller computing resources.) An improved discretization method has also been developed for staggered fermions (HISQ fermions) that substantially reduces discretization errors.

Using the resources of two supercomputing facilities has dramatically advanced research in this field and other strongly coupled field theories of importance to the study of high-energy and nuclear physics. This project's research results contribute to the DOE strategic goal of achieving major scientific discoveries by advancing fundamental knowledge in high-energy and nuclear physics that will result in a deeper understanding of matter, energy, space, and time.

Contributors/Authors

Paul B. Mackenzie, Fermi National Accelerator Laboratory

Principal Collaborators

The following are members of the Executive Committee of the U.S. Lattice Quantum Chromodynamics (USQCD) Collaboration, which oversees the lattice work at the ALCF and OLCF: Richard C. Brower, Boston University, head of the Software Committee; Norman H. Christ, Columbia University, a member of the Blue Gene/Q design team; Frithjof Karsch, Brookhaven National Laboratory, head of the Scientific Program Committee; Julius Kuti, UCSD; John W. Negele, Massachusetts Institute of Technology; David G. Richards, Jefferson Laboratory; Stephen R. Sharpe, University of Washington; and Robert Sugar, University of California—Santa Barbara, former principal investigator of USQCD.

Funding

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Publications

S.N. Syritsyn et al. 2010. "Nucleon Electromagnetic Form Factors from Lattice QCD Using 2+1 Flavor Domain Wall Fermions on Fine Lattices and Chiral Perturbation Theory." *Physical Review D* 81: 034507.

C. Bernard et al. 2009. "The $\bar{B} \to D^{*}\ell\bar{\nu}$ Form Factor at Zero Recoil from Three-Flavor Lattice QCD: A Model-Independent Determination of $|V_{cb}|$." *Physical Review D* 79: 014506.

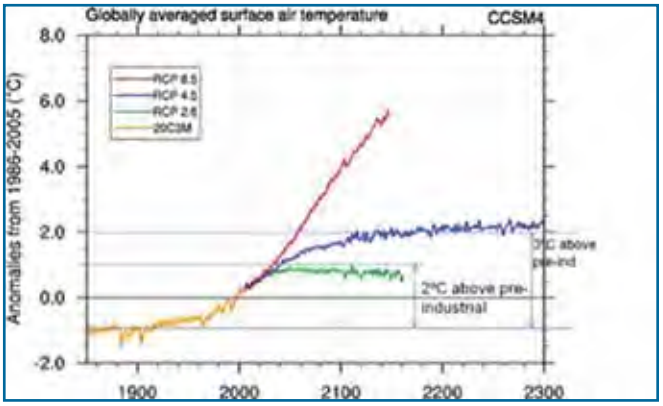
J. A. Bailey et al. 2009. "$B \to \pi\ell\nu$ Semileptonic Form Factor from Three-Flavor Lattice QCD: A Model-Independent Determination of $|V_{ub}|$." *Physical Review D* 79: 054507.

C. Allton et al. 2008. "Physical Results from 2+1 Flavor Domain Wall QCD and SU(2) Chiral Perturbation Theory." *Physical Review D* 78: 114509.

Computational End Station Provides Climate Data for IPCC Assessment Reports

ABSTRACT

Oak Ridge National Laboratory and Lawrence Berkeley National Laboratory provided more than half of the simulation data for the joint Department of Energy/National Science Foundation contribution to the Intergovernmental Panel on Climate Change Fourth Assessment Report, which concluded the Earth's climate is warming, probably due to human activities. By the end of 2010 Argonne National Laboratory and Oak Ridge National Laboratory supercomputers had generated data for model development and the panel's next assessment.



Shown are globally averaged surface air temperatures for a time series of CMIP5 runs (in progress) with CCSM4 at 1 degree resolution. Only emission profile, or representative concentration pathway (RCP), RCP2.6 keeps globally averaged temperatures less than 2 degrees Celsius above preindustrial (2081-2100 minus 1850-1900 = +1.83 degrees Celsius); RCP4.5 stabilizes temperatures about 3 degrees Celsius above preindustrial (Meehl et al. 2011).

Supercomputers serve as virtual time machines by running models and simulations that probe climate's past and present and simulate its future. The results inform policy, guide climate change strategy, and accelerate action to manage the changes. Led by Warren Washington of NSF's NCAR, INCITE projects at the ALCF and OLCF helped generate the largest set of publicly available climate change simulation data in the world for the IPCC Fourth Assessment Report, AR4, the most recent IPCC assessment report.

"Access to DOE high-performance computing assets at NERSC and leadership computing facilities at Oak Ridge and Argonne has significantly improved climate model simulations of the Earth's climate," Washington, an atmospheric scientist, said. "These computers made it possible to run more realistic physical processes at higher resolutions, with more ensemble members, and more historical (twentieth-century) validation simulations as well as extensive future climate scenarios. In fact, without the INCITE resources the United States would make a much smaller climate change research contribution to the science and policymaker community."

The project serves a broad DOE, NSF, and NASA climate science community. Its aim is to help develop and execute the next-generation CCSM, called the Community Earth System Model (CESM), that couples independent models describing Earth's atmosphere, oceans, land/vegetation, and sea ice. The effort contributes to the science missions of all three agencies. DOE, for example, wants to thoroughly understand consequences of energy use on present and future climate change.

The involved researchers have also developed a Climate-Science Computational End Station (CCES) to solve grand computational challenges in climate science. End-station users have continued to improve many aspects of the climate model and then use the newer model versions for studies of climate change with different emission scenarios that would result from adopting different energy policies. Climate community studies based on the project's simulations will improve the scientific basis, accuracy, and fidelity of climate models. Validating that models correctly depict Earth's past climate improves confidence that simulations can more accurately simulate future climate change. Some of the model versions have interactive biochemical cycles such as those of carbon or methane. A new DOE initiative for its laboratories and NCAR is Climate Science for a Sustainable Energy Future (CSSEF), which will accelerate development of a sixth-generation CESM. The CCES will directly support the CSSEF effort as one of its main priorities.

The CCES culminated the first stage of its development in 2010 with allocations of 70 million processor hours on ORNL's Jaguar Cray XT and 30 million processor hours on Argonne's IBM Blue Gene/P.

The CCES will advance climate science through both aggressive development of the model, such as the CSSEF, and creation of an extensive suite of climate simulations. Advanced computational simulation of the Earth system is built on a successful long-term interagency collaboration that includes NSF and most of the major DOE national laboratories in developing the CESM, NASA through its carbon data assimilation models, and university partners with expertise in computational climate research. Of particular importance is the improved simulation of the global carbon cycle and its direct and indirect feedbacks to the climate system, including its variability and modulation by ocean and land ecosystems.

The work indispensably benefits the larger climate science community striving to understand the interconnections underpinning climate change. For example, another INCITE project, led by Susan Kurien of LANL, aims to understand the influence of the ocean on climate. The project was allocated 25

million processor hours each year in 2009 and 2010 and 35 million processor hours in 2011 at the ALCF to study the effects of small-scale fluid dynamics, which are largely omitted from present climate models, on larger-scale resolved features such as global and regional ocean currents. It focuses on idealized systems with rotation and stratification parameters that are relevant to ocean and climate dynamics.

Washington and collaborators are now developing stage two of the CCES with a 2011 INCITE allocation of 70 million processor hours at the OLCF and 40 million at the ALCF. The work continues development and extensive testing of the CESM, a newer version of the CCSM that came into being in 2011.

Nobel past, challenging future

Through INCITE Washington and collaborators provided data for AR4, which concluded planetary warming during the twentieth century was probably the result of human activities. In 2004 and 2005 DOE supercomputers at ORNL and LBNL's NERSC provided more than half of the joint DOE/NSF data contribution to AR4. The DOE/NSF data contribution was put into a repository that scientists worldwide accessed to write approximately 300 journal articles cited in AR4. In 2007 the IPCC, which assesses climate change as described in peer-reviewed scientific publications, was awarded the Nobel Prize.

The CCES INCITE project will provide large amounts of climate model simulation data for the next IPCC report, AR5, expected in 2014. The CESM, which will probably generate the largest set of publicly available climate data to date, will enable comprehensive and detailed studies that will improve the level of certainty for IPCC conclusions.

The studies may improve our understanding of how components of the Earth system, such as ocean and atmosphere, affect each other. "The current state of the ocean depends on what has happened many years in the past, whereas the state of the atmosphere does not tend to depend on the past state for much more than weeks," said Phil Jones of LANL, who heads DOE's Climate, Ocean, and Sea Ice Modeling project to develop advanced ocean and ice models for evaluating high-latitude climate change. Jones is a coprincipal investigator on Washington's team to develop the CCES.

The atmosphere and ocean models solve fluid equations, while the sea-ice model solves equations pertaining to viscous plastics. The land-model equations focus on exchanges of moisture and heat across plant leaves and soil layers.

"We used to run the ocean model alone to look at ocean issues," Jones explained. "What we're doing now is running models coupled together. We're planning to run with a 25-kilometer resolution in the atmosphere and, in the ocean, 10 kilometers near the equator and a few kilometers near the Arctic. The sea ice tends to run on the ocean resolution, and the land can run on the atmosphere resolution."

Getting much more realism requires running simulations at the highest possible resolution. "That always requires more computing time," Jones said. Increasing resolution by a factor of two raises the calculating time by nearly an order of magnitude, he added. More grid points in the horizontal plane mean the supercomputer has to take smaller steps—and more computational time—to get to the same place.

High-resolution models help remove biases, where the modeled and observed states do not match. With lower-resolution models, the Gulf Stream has a strong bias for hugging the East Coast too long. The real Gulf Stream peels off the coast near Cape Hatteras in North Carolina. "That impacts where storm tracks go across the North Atlantic," Jones said.

The quest for greater realism in models requires ever more powerful supercomputers. Having learned a great deal about Earth's climate, past and present, from terascale and petascale systems, scientists look longingly to future exascale systems. A thousand times faster than today's quickest computers, exascale supercomputers may enable predictive computing and will certainly bring deeper understanding of the complex biogeochemical cycles that underpin global ecosystems and make life on Earth sustainable.

Contributors/Authors

Warren Washington, NCAR

Principal Collaborators

Washington collaborates with David Bader, John Drake, David Erickson, James Hack, and Peter Thornton, ORNL; Peter Gent, Lawrence Buja, James Hurrell, Jean-Francois Lamarque, and Bette Otto-Bliesner, NCAR; Phillip Cameron-Smith, Lawrence Livermore National Laboratory; Dave Considine and Steven Pawson, NASA; Steven Ghan and L. Ruby Leung, PNNL; Scott Elliott and Philip Jones, LANL; Robert Jacob, Argonne; and Mark Taylor, Sandia. The coordinator is Tom Bettge, NCAR.

Funding

DOE, NSF, and NASA

Publications

W. Washington et al. 2009. "How Much Climate Change Can Be Avoided by Mitigation?" *Geophysical Research Letters* 36, L08703.

W. Washington, L. Buja, and A. Craig. 2009. "The Computational Future for Climate and Earth System Models: On the Path to Petaflop and Beyond." *Philosophical Transactions of the Royal Society A-Mathematical Physical and Engineering Sciences* 367, no. 1890: 833–846.

D. Kerbyson and P. Jones. 2005. "A Performance Model of Parallel Ocean Program." *Journal of High Performance Computing Applications* 19, no. 3: 261–276.

List of Abbreviations

2D—two-dimensional

3D—three-dimensional

ADIOS—Adaptive Input/Output System

AIDS—acquired immune deficiency syndrome

ALCF—Argonne Leadership Computing Facility

ARRA—American Recovery and Reinvestment Act of 2009

Argonne—Argonne National Laboratory

ASCR—Advanced Scientific Computing Research (DOE program)

ATP—adenosine triphosphate

CCES—Climate-Science Computational End Station

CCSM—Community Climate System Model

CESM—Community Earth System Model

CERFACS—Center for Research and Formation for Advanced Scientific Computations

CFD—computational fluid dynamics

CPU—central processing unit

CCSEF—Climate Science for a Sustainable Energy Future

CTR—Center for Turbulence Research

DNA— deoxyribonucleic acid

DNS—direct numerical simulation

DOE—Department of Energy

ETH Zürich—Eidgenössische Technische Hochschule Zürich

GCD—gravitationally confined detonation

GPU—graphics processing unit

HPC—high-performance computing

GFDL—Geophysical Fluid Dynamics Laboratory

I/O—input/output

INCITE—Innovative and Novel Computational Impact on Theory and Experiment

INL—Idaho National Laboratory

IPCC—Intergovernmental Panel on Climate Change

LANL—Los Alamos National Laboratory

LBNL—Lawrence Berkeley National Laboratory

LCF—Leadership Computing Facility

LES—large eddy simulation

LLNL—Lawrence Livermore National Laboratory

MD—molecular dynamics

MFDn —Many Fermion Dynamics-nuclear

NASA—National Aeronautics and Space Administration

NCAR—National Center for Atmospheric Research

NEAMS—Nuclear Energy Advanced Modeling and Simulation

NEMO—Nanoelectric Modeling

NERSC—National Energy Research Scientific Computing Center

NIST—National Institute of Standards and Technology

NMR—nuclear magnetic resonance

NNSA—National Nuclear Security Administration

NOAA—National Oceanic and Atmospheric Administration

NSF—National Science Foundation

OLCF—Oak Ridge Leadership Computing Facility

ORNL—Oak Ridge National Laboratory

PCNA—proliferating cell nuclear antigen

PNNL—Pacific Northwest National Laboratory

PPPL—Princeton Plasma Physics Laboratory

QCD—quantum chromodynamics

QM—quantum mechanical

R&D—research and development

RANS—Reynolds-averaged Navier-Stokes

Sandia—Sandia National Laboratories

SASI—standing accretion shock instability

SCC—stress corrosion cracking

SCEC—Southern California Earthquake Center

SciDAC—Scientific Discovery through Advanced Computing (DOE program)

SDSC—San Diego Supercomputer Center

SDSU—San Diego State University

SHARP—Simulation-Based High-Efficiency Advanced Reactor Prototyping

UCLA—University of California–Los Angeles

UCSC—University of California–Santa Cruz

UCSD—University of California−San Diego

USC—University of Southern California

USQCD—U.S. Lattice Quantum Chromodynamics (a collaboration)

ZPG—zero pressure gradient

Appendix

2011 INCITE Awards

"Ab Initio Dynamical Simulations for the Prediction of Bulk Properties"
Principal Investigator: Theresa Windus, Iowa State University
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Advanced Reactor Thermal Hydraulic Modeling"
Principal Investigator: Paul F. Fischer, Argonne
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond"
Principal Investigator: William M. Tang, Princton University
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Cellulosic Ethanol: Simulation of Multicomponent Biomass System"
Principal Investigator: Jeremy Smith, ORNL
30,000,000 processor hours, Cray XT, ORNL

"CHiMES: Coupled High-resolution Modeling of the Earth System"
Principal Investigator: Venkatramani Balaji, NOAA
20,000,000 processor hours, Cray XT, ORNL

"Climate-Science Computational Development Team: The Climate End Station II"
Principal Investigator: Warren Washington, NCAR
110,000,000 processor hours, IBM Blue Gene/P, Argonne (40,000,000 processor hours); Cray XT, ORNL (70,000,000 processor hours)

"Coarse Grained Molecular Dynamics Studies of Vesicle Formation and Fusion"
Principal Investigator: Michael Klein, Temple University
30,000,000 processor hours, Cray XT, ORNL

"Control of Complex Transformations with Advanced Molecular Simulation Methods"
Principal Investigator: Christopher Mundy, PNNL
20,000,000 processor hours, Cray XT, ORNL

"Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders"
Principal Investigator: Philippe Spalart, The Boeing Company
45,000,000 processor hours, IBM Blue Gene/P, Argonne

"Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz"
Principal Investigator: Thomas H. Jordan, USC
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Electronic Structure Calculations for Nanostructures"
Principal Investigator: Lin-Wang Wang, LBNL
10,000,000 processor hours, Cray XT, ORNL

"Explosive Hazard Predictions with the Uintah Framework"
Principal Investigator: Martin Berzins, University of Utah
15,000,000 processor hours, Cray XT, ORNL

"Gyrokinetic Simulation of Energetic Particle Turbulence in ITER Burning Plasmas"
Principal Investigator: Zhihong Lin, University of California-Irvine
35,000,000 processor hours, Cray XT, ORNL

"High-Fidelity Simulations for Advanced Engine Combustion Research"
Principal Investigator: Joseph Oefelein, Sandia; Ramanan Sankaran, ORNL
60,000,000 processor hours, Cray XT, ORNL

"High Fidelity Simulation of Complex Suspension Flow for Practical Rheometry"
Principal Investigator: William George, NIST
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"High Fidelity Tokamak Edge Simulation for Efficient Confinement of Fusion Plasma"
Principal Investigator: C.S. Chang, New York University
50,000,000 processor hours, Cray XT, ORNL

"How High Redshift Galaxies Reionized the Universe"
Principal Investigator: Michael Norman, UCSD
35,000,000 processor hours, Cray XT, ORNL

"Investigation of Multi-Scale Transport Physics of Fusion Experiments Using Global Gyrokinetic Turbulence Simulations"
Principal Investigator: Weixing Wang, PPPL
20,000,000 processor hours, Cray XT, ORNL

"Large Eddy Simulation for Green Energy and Propulsion Systems"
Principal Investigator: Umesh Paliath, GE Global Research
20,000,000 processor hours, IBM Blue Gene/P, Argonne

"Large Eddy Simulation of Two Phase Flow Combustion in Gas Turbines"
Principal Investigator: Thierry Poinsot, CERFACS
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Lattice QCD"
Principal Investigator: Paul B. Mackenzie, Fermi National Accelerator Laboratory
50,000,000 processor hours, IBM Blue Gene/P, Argonne; 30,000,000 processor hours, Cray XT, ORNL

"Multiscale Blood Flow Simulations"
Principal Investigator: George Karniadakis, Brown University
50,000,000 processor hours, IBM Blue Gene/P, Argonne

"Nuclear Structure and Nuclear Reactions"
Principal Investigator: James Vary, Iowa State University
28,000,000 processor hours, Cray XT, ORNL; 15,000,000 processor hours, IBM Blue Gene/P, Argonne

"Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence"
Principal Investigator: Susan Kurien, LANL
35,000,000 processor hours, IBM Blue Gene/P

"Performance Evaluation and Analysis Consortium End Station"
Principal Investigator: Patrick Worley, ORNL
20,000,000, Cray XT, ORNL; 10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Modeling of Chemical Catalysts and Interfaces"
Principal Investigator: Robert Harrison, ORNL
75,000,000 processor hours, Cray XT, ORNL

"Petascale Modeling of Nano-electronic Devices"
Principal Investigator: Gerhard Klimeck, Purdue University
15,000,000 processor hours, Cray XT, ORNL

"Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Principal Investigator: Warren Mori, UCLA
12,000,000 processor hours, Cray XT, ORNL

"Petascale Simulations of Stress Corrosion Cracking"
Principal Investigator: Priya Vashishta, USC
45,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Simulations of Type 1a Supernovae from Ignition to Observables"
Principal Investigator: Stan Woosley, UCSC
50,000,000 processor hours, Cray XT, ORNL

"Potential Energy Surfaces for Simulating Complex Chemical Processes"
Principal Investigator: Donald G. Truhlar, University of Minnesota
15,000,000 processor hours, IBM Blue Gene/P, Argonne

"Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculation"
Principal Investigator: Jeffrey Greeley, Argonne
15,000,000 processor hours, IBM Blue Gene/P, Argonne

"Protein-Ligand Interaction Simulations and Analysis"
Principal Investigator: T. Andrew Binkowski, Argonne
20,000,000 processor hours, IBM Blue Gene/P, Argonne

"Quantum Monte Carlo Brings New Realism to Surface-Science Modeling"
Principal Investigator: Dario Alfè, University College London
17,000,000 processor hours, Cray XT, ORNL

"Quantum Monte Carlo Simulation of Models of Condensed Matter"
Principal Investigator: Richard Needs, University of Cambridge
15,000,000 processor hours, Cray XT, ORNL

"Scalable System Software for Performance and Productivity"
Principal Investigator: Ewing Lusk, Argonne
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Sculpting Biological Membranes by Proteins"
Principal Investigator: Klaus Schulten, University of Illinois, Urbana-Champaign
5,000,000 processor hours, Cray XT, ORNL

"Simulation of High Reynolds Number Turbulent Boundary Layers"
Principal Investigator: Robert Moser, University of Texas at Austin
40,000,000 processor hours, IBM Blue Gene/P, Argonne

"Simulation and Modeling of Membranes' Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions"
Principal Investigator: Igor Tsigelny, UCSD
4,000,000 processor hours, IBM Blue Gene/P, Argonne

"Simulation of Turbulent Lean Hydrogen Flames in High Pressure"
Principal Investigator: John Bell, LBNL
40,000,000 processor hours, Cray XT, ORNL

"Simulations of Deflagration-to-Detonation Transition in Reactive Gases"
Principal Investigator: Alexei Khokhlov, University of Chicago
18,000,000 processor hours, IBM Blue Gene/P, Argonne

"Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond"
Principal Investigator: Denise Hinkel, LLNL
50,000,000 processor hours, IBM Blue Gene/P, Argonne

"Singularities and Multi-Scaling in MHD"
Principal Investigator: Annick Pouquet, NCAR
15,000,000 processor hours, Cray XT, ORNL

"Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models"
Principal Investigator: Don Lamb, University of Chicago ASC FLASH Center
80,000,000 processor hours, IBM Blue Gene/P, Argonne

"Three Dimensional Simulations for Core Collapse Supernovae"
Principal Investigator: Anthony Mezzacappa, ORNL
60,000,000 processor hours, Cray XT, ORNL

"Towards Breakthroughs in Protein Structure Calculation and Design"
Principal Investigator: David Baker, University of Washington
30,000,000 processor hours, IBM Blue Gene/P, Argonne

"Trace Collection for Simulation-Driven Co-Design of Exascale Platforms and Codes"
Principal Investigator: David Evensky, Sandia
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Turbulent Heating of Astrophysical Plasma"
Principal Investigator: Gregory Howes, University of Iowa
10,000,000 processor hours, Cray XT, ORNL

"Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability"
Principal Investigator: Sanjiva Lele, Stanford University
12,000,000 processor hours, IBM Blue Gene/P, ORNL

"Ultrascale Simulation of Basin-Scale CO2 Sequestration in Deep Geologic Formations and Radionuclide Migration using PFLOTRAN"
Principal Investigator: Peter Lichtner, LANL
15,000,000 processor hours, Cray XT, ORNL

"Uncertainty Quantification for Three-Dimensional Reactor Assembly Simulations"
Principal Investigator: Thomas Evans, ORNL
18,000,000 processor hours, Cray XT, ORNL

"Uncertainty Quantification for Turbulent Mixing"
Principal Investigator: James G. Glimm, State University of New York, Stony Brook
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air"
Principal Investigator: Jack Wells, ORNL
25,000,000 processor hours, IBM Blue Gene/P, Argonne; 10,000,000 processor hours, Cray XT, ORNL

"Unraveling the Physics of Magnetic Reconnection with 3D Kinetic Simulations"
Principal Investigator: William Daughton, LANL
30,000,000 processor hours, Cray XT, ORNL

"Validation of Plasma Microturbulence Simulations for Finite-Beta Fusion Experiments"
Principal Investigator: William Nevins, LLNL
20,000,000 processor hours, Cray XT, ORNL

"Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces"
Principal Investigator: Giulia Galli, University of California, Davis
15,000,000 processor hours, IBM Blue Gene/P, Argonne

2010 INCITE Awards

"Advanced Reactor Thermal Hydraulic Modeling"
Principal Investigator: Paul Fischer, Argonne
32,000,000 processor hours, IBM Blue Gene/P, Argonne; 2,000,000 processor hours, Cray XT, ORNL

"Assessing Transient Global Climate Response Using the NCAR-CCSM3: Climate Sensitivity and Abrupt Climate Change"
Principal Investigator: Zhengyu Liu, University of Wisconsin–Madison
5,000,000 processor hours, Cray XT, ORNL

"BG/P Plan 9 Measurements on Large Scale Systems"
Principal Investigator: Ronald Minnich, Sandia
1,000,000 processor hours, IBM Blue Gene/P, Argonne

"Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"
Principal Investigator: Jeremy Smith, ORNL
25,000,000 processor hours, Cray XT, ORNL

"CHiMES: Coupled High-Resolution Modeling of the Earth System"
Principal Investigator: Venkatramani Balaji, NOAA/ GFDL
20,000,000 processor hours, Cray XT, ORNL

"Clean and Efficient Coal Gasifier Designs Using Large-Scale Simulations"
Principal Investigator: Madhava Syamlal, DOE, National Energy Technology Laboratory
6,000,000 processor hours, Cray XT, ORNL

"Climate-Science Computational End Station Development and Grand Challenge Team"
Principal Investigator: Warren Washington, NCAR
100,000,000 processor hours, Cray XT, ORNL; 30,000,000 processor hours, IBM Blue Gene/P, Argonne

"Computational Nuclear Structure"
Principal Investigator: David Dean, ORNL
40,000,000 processor hours, Cray XT, ORNL; 15,000,000 processor hours, IBM Blue Gene/P, Argonne

"Computational Protein Structure Prediction and Protein Design"
Principal Investigator: David Baker, University of Washington
50,000,000 Processor hours, IBM Blue Gene/P, Argonne

"Computational Surface Science at High Accuracy with Quantum Monte Carlo"
Principal Investigator: Dario Alfè, University College London
20,000,000 processor hours, Cray XT, ORNL

"Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz"
Principal Investigator: Thomas Jordan, Southern California Earthquake Center
27,000,000 processor hours, Cray XT, ORNL; 7,000,000 processor hours, IBM Blue Gene/P, Argonne

"Development and Correlations of Computational Tools for Transport Airplanes"
Principal Investigator: Moeljo Hong, the Boeing Company
6,000,000 processor hours, Cray XT, ORNL

"Electronic, Lattice, and Mechanical Properties of Novel Nano-Structured Bulk Materials"
Principal Investigator: Jihui Yang, General Motors Research and Development Center
14,000,000 processor hours, Cray XT, ORNL

"Electronic Structure Calculations of Nano Solar Cells"
Principal Investigator: Lin-Wang Wang, LBNL
9,000,000 processor hours, Cray XT, ORNL; 1,000,000 processor hours, IBM Blue Gene/P,
Argonne

"Gyrokinetic Simulation of Energetic Particle Turbulence in ITER Burning Plasmas"
Principal Investigator: Zhihong Lin, University of California–Irvine
20,000,000 processor hours, Cray XT, ORNL

"High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels"
Principal Investigator: Jacqueline Chen and Joseph Oefelein, Sandia
65,000,000 processor hours, Cray XT, ORNL; 2,000,000 processor hours, IBM Blue Gene/P, Argonne

"High-Fidelity Tokamak Edge Simulation for Efficient Confinement of Fusion Plasma"
Principal Investigator: C. S. Chang, New York University
50,000,000 processor hours, Cray XT, ORNL

"High Resolution Ensemble Simulations of Hurricanes"
Principal Investigator: Robert Gall, NOAA
20,000,000 processor hours, Cray XT, ORNL

"High Resolution Global Simulation of Plasma Microturbulence"
Principal Investigator: William Tang, PPPL
12,000,000 Processor Hours, IBM Blue Gene/P, Argonne

"HPC Colony: Removing Scalability, Fault, and Performance Barriers in Leadership Class Systems through Adaptive System Software"
Principal Investigator: Terry Jones, ORNL
4,000,000 processor hours, Cray XT, ORNL

"An Integrated Approach to the Rational Design of Chemical Catalysts"
Principal Investigator: Robert Harrison, ORNL
75,000,000 processor hours, Cray XT, ORNL

"Interaction of Turbulence and Chemistry in Lean Premixed Laboratory Flames"
Principal Investigator: John Bell, LBNL
8,000,000 processor hours, Cray XT, ORNL

"Interplay of AAA+ Molecular Machines, DNA Repair Enzymes, and Sliding Clamps at the Replication Fork: A Multiscale Approach to Modeling Replisome Assembly and Function"
Principal Investigator: Ivaylo Ivanov, UCSD and Howard Hughes Medical Institute
4,000,000 processor hours, Cray XT, ORNL

"Investigation of Multi-Scale Transport Physics of Fusion Experiments Using Global Gyrokinetic Turbulence Simulations"
Principal Investigator: Weixing Wang, PPPL
34,000,000 processor hours, Cray XT, ORNL

"Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles"
Principal Investigator: Christopher Wolverton, Northwestern University
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Large Eddy Simulation of Two Phase Flow Combustion in Gas Turbines"
Principal Investigator: Thierry Poinsot, CERFACS
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Large Scale Condensed Matter and Fluid Dynamics Simulations"
Principal Investigator: Peter Coveney, University College London
40,000,000 processor hours, Blue Gene/P, Argonne

"Lattice QCD"
Principal Investigator: Paul Mackenzie, Fermi National Accelerator Laboratory
67,000,000 processor hours, IBM Blue Gene/P, Argonne; 40,000,000 processor hours, Cray XT, ORNL

"Magnetic Structure and Thermodynamics of Low Dimensional Magnetic Structures"
Principal Investigator: Markus Eisenbach, ORNL
21,000,000 processor hours, Cray XT, ORNL

"Millisecond Molecular Dynamics of Chaperoning of Unfolded Polypeptide Chains by HSP70"
Principal Investigator: Harold Scheraga, Cornell University
6,000,000 processor hours, IBM Blue Gene/P, Argonne

"Modeling the Rheological Properties of Concrete"
Principal Investigator: William George. NIST
2,000,000 processor hours, IBM Blue Gene/P, Argonne

"Molecular Simulation of Complex Chemical Systems" Principal Investigator: Christopher Mundy, PNNL
10,000,000 processor hours, Cray XT ORNL; 2,000,000 processor hours, IBM Blue Gene/P, Argonne

"Multidimensional Models of Type Ia Supernovae from Ignition to Observables"
Principal Investigator: Stan Woosley, UCSC
5,000,000 processor hours, Cray XT, ORNL

"Multidimensional Simulations of Core Collapse Supernovae"
Principal Investigator: Anthony Mezzacappa, ORNL
34,000,000 processor hours, Cray XT, ORNL

"Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials"
Principal Investigator: Mark Jarrell, Louisiana State University
17,000,000 processor hours, Cray XT, ORNL

"Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence"
Principal Investigator: Susan Kurien, LANL
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"Overcoming the Turbulent-Mixing Characterization Barrier to Green Energy and Propulsion Systems"
Principal Investigator: Anurag Gupta, General Electric Global Research
19,000,000 processor hours, IBM Blue Gene/P, Argonne

"Performance Evaluation and Analysis Consortium End Station"
Principal Investigator: Patrick Worley, ORNL
20,000,000 processor hours, Cray XT, ORNL; 8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Adaptive Computational Fluid Dynamics for Applications with High Anisotropy"
Principal Investigator: Kenneth Jansen, Rensselaer
10,000,000 processor hours, IBM Blue Gene/P, Argonne; 10,000,000 processor hours, Cray XT, ORNL

"Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling"
Principal Investigator: Lie-Quan Lee, SLAC National Accelerator Laboratory
12,000,000 processor hours, Cray XT, ORNL

"Petascale Modeling of Nano-Electronic Devices"
Principal Investigator: Gerhard Klimeck, Purdue University
18,000,000 processor hours, Cray XT, ORNL

"Petascale Particle-in-Cell Simulations of Fast Ignition"
Principal Investigator: John Tonge, UCLA
7,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Principal Investigator: Warren Mori, UCLA
8,000,000 processor hours, Cray XT, ORNL

"A Petascale Study of Turbulent Mixing in Non-Stratified and Stratified Flows"
Principal Investigator: Pui-kuen Yeung, Georgia Institute of Technology
20,000,000 processor hours, Cray XT, ORNL

"Prediction of Bulk Properties Using high Accuracy Ab Initio Methods Interfaced with Dynamical Calculations"
Principal Investigator: Theresa Windus, Ames Laboratory
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Predictions of Thermal Striping in Sodium Cooled Reactors"
Principal Investigator: Andrew Siegel, Argonne
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Predictive and Accurate Monte Carlo Based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems"
Principal Investigator: Thomas C. Schulthess, Swiss National Supercomputing Centre
70,000,000 processor hours, Cray XT, ORNL

"Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations"
Principal Investigator: Jeffrey Greeley, Argonne
10,000,000 processor hours, IBM Blue Gene/P, Argonne

"Protein-Ligand Interaction Simulations and Analysis"
Principal Investigator: T. Andrew Binkowski, Argonne
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"Quantum Simulations of Nanostructural Materials for Renewable Energy Applications"
Principal Investigator: Giulia Galli, University of California, Davis
1,000,000 processor hours, IBM Blue Gene/P, Argonne

"Research into the Systematics of Type Ia Supernovae"
Principal Investigator: Alan Calder, Stony Brook University
35,000,000 processor hours, IBM Blue Gene/P, Argonne

"Scalable System Software for Performance and Productivity"
Principal Investigator: Ewing Lusk, Argonne
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Scalable System Software Research for Extreme-Scale Computing"
Principal Investigator: Ron Oldfield, Sandia
5,000,000 processor hours, Cray XT, ORNL

"Sculpting Biological Membranes by Proteins"
Principal Investigator: Klaus Schulten, University of Illinois–Urbana-Champaign
25,000,000 processor hours, Cray XT, ORNL

"Sequencing DNA using MspA"
Principal Investigator: Aleksei Aksimentiev, University of Illinois–Urbana-Champaign
10,000,000 processor hours, Cray XT, ORNL

"Simulation of Global Cloudiness"
Principal Investigator: David Randall, Colorado State University
3,000,000 processor hours, Cray XT, ORNL

"Simulation of 'High' Reynolds Number Turbulent Boundary Layers"
Principal Investigator: Robert Moser, University of Texas at Austin
33,000,000 processor hours, IBM Blue Gene/P, Argonne

"Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions"
Principal Investigator: Igor Tsigelny, UCSD
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond"
Principal Investigator: Denise Hinkel, LLNL
45,000,000 processor hours, IBM Blue Gene/P, Argonne

"Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models"
Principal Investigator: Don Lamb, University of Chicago ASC FLASH Center
70,000,000 Processor hours, IBM Blue Gene/P, Argonne

"Turbulent Heating of Astrophysical Plasmas"
Principal Investigator: Gregory Howes, University of Iowa
12,000,000 processor hours, Cray XT, ORNL

"Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability"
Principal Investigator: Sanjiva Lele, Stanford University
12,000,000 processor hours, IBM Blue Gene/P, Argonne

"Ultrascale Simulation of Basin-Scale CO2 Sequestration in Deep Geologic Formations and Radionuclide Migration using PFLOTRAN"
Principal Investigator: Peter Lichtner, LANL
18,000,000 processor hours, Cray XT, ORNL

"Unbalanced Magnetohydrodynamic Turbulence"
Principal Investigator: Stanislav Boldyrev, University of Wisconsin-Madison
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"Uncertainty Quantification for Three-Dimensional Reactor Assembly Simulations"
Principal Investigator: Thomas Evans, ORNL
8,000,000 processor hours, Cray XT, ORNL

"Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air"
Principal Investigator: Jack Wells, ORNL
12,000,000 processor hours, IBM Blue Gene/P, Argonne; 12,000,000 processor hours, Cray XT, ORNL

"Validation of Plasma Microturbulence Simulations for Finite-Beta Fusion Experiments"
Principal Investigator: William Nevins, LLNL
30,000,000 processor hours, Cray XT, ORNL

"Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas"
Principal Investigator: Patrick Diamond, UCSD and Howard Hughes Medical Institute
35,000,000 processor hours, Cray XT, ORNL

"The Via Lactea Project: A Glimpse into the Invisible World of Dark Matter"
Principal Investigator: Piero Madau, UCSC
5,000,000 processor hours, Cray XT, ORNL

2009 INCITE Awards

"CHiMES: Coupled High-resolution Modeling of the Earth System"
Principal Investigator: Venkatramani Balaji, NOAA / GFDL
24,000,000 processor hours, Cray XTs, ORNL

"Integrated Simulations of Energetic Particles Driven by High Power Electromagnetic Waves in Fusion Plasmas"
Principal Investigator: Paul Bonoli, Plasma Science and Fusion Center
5,000,000 processor hours, NERSC HPC, NERSC

"The Role of Eddies in the Meridional Overturning Circulation"
Principal Investigator: Paola Cessi, Scripps Institution of Oceanography/UCSD
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"High-Fidelity Tokamak Edge Simulation for Efficient Confinement of Fusion Plasma"
Principal Investigator: C.S. Chang, New York University
20,000,000 processor hours, Cray XTs, ORNL

"Surface Input Reanalysis for Climate Applications (SIRCA) 1850-2011"
Principal Investigator: Gilbert Compo, University of Colorado/CIRES/Climate Diagnostics Center and NOAA Earth System Research Laboratory/PSD
1,100,000 processor hours, Cray XTs, ORNL

"Large Scale Condensed Matter and Fluid Dynamics Simulations"
Principal Investigator: Peter Coveney, University College London
40,000,000 processor hours, IBM Blue Gene/P, Argonne

"Massively Parallel Simulation of Pump-Probe Time-Resolved Photoemission"
Principal Investigator: James Freericks, Georgetown University
2,250,000 processor Hours, NERSC HPC (2,250,000 processor hours)

"High Fidelity Computations for Complex Biological Membranes"
Principal Investigator: Michael Heroux, Sandia
1,000,000 processor hours, Cray XTs, ORNL

"Development and Correlations of Computational Tools for transport Airplanes"
Principal Investigator: Moeljo Hong, the Boeing Co.
1,000,000 processor hours, Cray XTs,

"Interplay of AAA+ Molecular Machines, DNA Repair Enzymes and Sliding Clamps at the Replication Fork: A Multiscale Approach to Modeling Replisome Assembly and Function"
Principal Investigator: Ivaylo Ivanov, UCSD and Howard Hughes Medical Institute
2,600,000 processor hours, Cray XTs, ORNL

"Petascale Adaptive CFD for Anisotropic Flows"
Principal Investigator: Kenneth Jansen, Rensselaer Polytechnic Institute
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz"
Principal Investigator: Thomas Jordan, Southern California Earthquake Center
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Simulations of Nano-electronic Devices"
Principal Investigator: Gerhard Klimeck, Purdue University
5,000,000 processor hours, Cray XTs, ORNL

"Intermittency and Star Formation in Turbulent Molecular Clouds"
Principal Investigator: Alexei Kritsuk, UCSD
5,000,000 processor hours, Cray XTs, ORNL

"Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence"
Principal Investigator: Susan Kurien, LANL
25,000,000 processor hours, IBM Blue Gene/P, Argonne

"Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models"
Principal Investigator: Don Lamb, University of Chicago ASC FLASH Center
70,000,000 processor hours, IBM Blue Gene/P, Argonne

"Fundamental Study of Shock/Turbulence Interaction"
Principal Investigator: Sanjiva Lele, Stanford University
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Assessing Transient Global Climate Response using the NCARCCSM3: Climate Sensitivity and Abrupt Climate Change"
Principal Investigator: Zhengyu Liu, University of Wisconsin, Madison
4,000,000 processor hours, Cray XTs, ORNL

"The Via Lactea Project: A Glimpse into the Invisible World of Dark Matter"
Principal Investigator: Piero Madau, UCSC
5,000,000 processor hours, Cray XTs, ORNL

"Propulsor Analyses for a Greener, High Bypass Ratio, Aircraft Gas Turbine Engine"
Principal Investigator: Robert Malecki, Pratt & Whitney
1,500,000 processor hours, Cray XTs, ORNL

"Structural and Dynamical Studies of Hydronium and Hydroxide ions in Bulk Water and at the Water/Air Interface Using Ab Initio Path Integral Simulations"
Principal Investigator: Thomas Miller, California Institute of Technology
12,000,000 processor hours, Cray XTs, ORNL

"Validation of Plasma Microturbulence Simulations for Finite-Beta Fusion Experiments"
Principal Investigator: William Nevins, LLNL
20,000,000 processor hours, Cray XTs, ORNL

"Dynamically Tunable Ferroelectric Surface Catalysts"
Principal Investigator: Andrew Rappe, University of Pennsylvania
2,283,200 processor hours, Cray XTs, ORNL

"Sculpting Biological Membranes by Proteins"
Principal Investigator: Klaus Schulten, University of Illinois
9,240,000 processor hours, IBM Blue Gene/P, Argonne

"Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions"
Principal Investigator: Igor Tsigelny, UCSD
3,000,000 processor hours, IBM Blue Gene/P, Argonne

"Molecular Simulations of Surfactant Assisted Aqueous Foam Formation"
Principal Investigator: Kelly Anderson, Procter and Gamble
6,000,000 processor hours, IBM Blue Gene/P, Argonne

"Computational Protein Structure Prediction and Protein Design"
Principal Investigator: David Baker, University of Washington
12,000,000 processor hours, IBM Blue Gene/P, Argonne

"Interaction of Turbulence and Chemistry in Lean Premixed Laboratory Flames"
Principal Investigator: John Bell, LBNL
3,000,000 processor hours, NERSC HPC, NERSC

"Gyrokinetic Steady State Transport Simulations"
Principal Investigator: Jeff Candy, General Atomics
2,000,000 processor hours, Cray XTs, ORNL

"Numerical Relativity Simulations of Binary Black Holes and Gravitational Radiation"
Principal Investigator: Joan Centrella, NASA Goddard Space Flight Center
500,000 processor hours, Cray XTs, ORNL

"Computational Rheology of Dense Suspensions"
Principal Investigator: Athonu Chatterjee, Corning Inc.
1,600,000 processor hours, HP-MPP, PNNL

"High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels"
Principal Investigator: Jacqueline Chen, Sandia
30,000,000 processor hours, Cray XTs, ORNL

"Computational Nuclear Structure"
Principal Investigator: David Dean, ORNL
10,000,000 processor hours, IBM Blue Gene/P, Argonne; 15,000,000 processor hours, Cray XTs, ORNL

"Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas"
Principal Investigator: Patrick Diamond, UCSD
30,000,000 processor hours, Cray XTs, ORNL

"Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows"
Principal Investigator: Hermann Fasel, University of Arizona
500,000 processor hours, Cray XTs, ORNL

"Reactor Core Hydrodynamics"
Principal Investigator: Paul Fischer, Argonne
30,000,000 processor hours, IBM Blue Gene/P, Argonne

"Large-Scale Simulations of Cardiac Electrical Activity"
Principal Investigator: Jeffrey Fox, Gene Network Sciences
21,405,500 processor hours, IBM Blue Gene/P, Argonne

"Water in Confined States"
Principal Investigator: Giulia Galli, University of California, Davis
2,000,000 processor hours; IBM Blue Gene/P, Argonne

"Modeling the Rheological Properties of Concrete"
Principal Investigator: William George, NIST
750,000 Processor Hours, IBM Blue Gene/P, Argonne

"An Integrated Approach to the Rational Design of Chemical Catalysts"
Principal Investigator: Robert Harrison, ORNL
30,000,000 processor hours, Cray XTs, ORNL

"High Power Electromagnetic Wave Heating in the ITER Burning Plasma"
Principal Investigator: E. Fred Jaeger, ORNL
2,000,000 processor hours, Cray XTs, ORNL

"Understanding the Electronic Structure of Novel Electronic Materials Using Many-Body Perturbation Theory"
Principal Investigator: Leeor Kronik, Weizmann Institute of Science
810,000 processor hours, NERSC HPC, NERSC

"Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling"
Principal Investigator: Lie-Quan Lee, SLAC National Accelerator Laboratory
8,000,000 processor hours, Cray XTs, ORNL

"Modeling Reactive Flows in Porous Media"
Principal Investigator: Peter Lichtner, LANL
10,000,000 processor hours, Cray XTs, ORNL; 500,000 processor hours,HP-MPP, PNNL

"Multidimensional Simulations of Core Collapse Supernovae"
Principal Investigator: Anthony Mezzacappa, ORNL
75,000,000 processor hours, Cray XTs, ORNL

"BG/P Plan 9 Measurements on Large Scale Systems"
Principal Investigator: Ronald Minnich, Sandia
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Principal Investigator: Warren Mori, UCLA
4,600,000 processor hours, NERSC HPC, NERSC

"Molecular Simulation of Complex Chemical Systems"
Principal Investigator: Christopher Mundy, PNNL
2,000,000 processor hours, IBM Blue Gene/P, Argonne; 2,000,000 processor hours, Cray XTs, ORNL

"Massively Parallel Simulation of Combustion in Gas Turbines"
Principal Investigator: Thierry Poinsot, CERFACS
8,000,000 processor hours, IBM Blue Gene/P, Argonne

"Beam Delivery System Optimization for X-Ray Free Electron Lasers"
Principal Investigator: Ji Qiang, LBNL
800,000 processor hours, NERSC HPC, NERSC

"Simulation of Global Cloudiness"
Principal Investigator: David Randall, Colorado State University
2,000,000 processor hours, Cray XTs, ORNL

"Three-Dimensional Particle-in-Cell Simulations of Fast Ignition"
Principal Investigator: Chuang Ren, University of Rochester
1,500,000 processor hours, IBM Blue Gene/P, Argonne; 1,000,000 processor hours, NERSC HPC, NERSC

"Bose-Einstein Condensation vs. Quantum Localization in Quantum Magnets"
Principal Investigator: Tommaso Roscilde, Ecole Normale Superieure de Lyon
1,200,000 processor hours, Cray XTs, ORNL

"Gating Mechanism of Membrane Proteins"
Principal Investigator: Benoit Roux, Argonne/University of Chicago
30,000,000 processor hours, IBM Blue Gene/P, Argonne; 15,000,000 processor hours, Cray XTs, ORNL

"Predictive and Accurate Monte Carlo Based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems"
Principal Investigator: Thomas Schulthess, ORNL
45,000,000 processor hours, Cray XTs, ORNL

"Predictions of Thermal Striping in Sodium Cooled Reactors"
Principal Investigator: Andrew Siegel, Argonne
7,500,000 processor hours, IBM Blue Gene/P, Argonne

"Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"
Principal Investigator: Jeremy Smith, ORNL
6,000,000 Processor Hours, Cray XTs, ORNL

"Lattice QCD"
Principal Investigator: Paul Mackenzie, Fermi National Accelerator Laboratory
67,000,000 processor hours, IBM Blue Gene/P, Argonne; 20,000,000 processor hours, Cray XTs, ORNL

"Clean and Efficient Coal Gasifier Designs using Large-Scale Simulations"
Principal Investigator: Madhava Syamlal, National Energy Technology Laboratory
13,000,000 processor hours, Cray XTs, ORNL

"High Resolution Global Simulation of Plasma Microturbulence"
Principal Investigator: William Tang, PPPL
6,000,000 processor hours, IBM Blue Gene/P, Argonne

"Linear Scale Electronic Structure Calculations for Nanostructures"
Principal Investigator: Lin-Wang Wang, LBNL
1,000,000 processor hours, IBM Blue Gene/P, Argonne; 2,000,000 processor hours, Cray XTs, ORNL

"Climate-Science Computational End Station Development and Grand Challenge Team"
Principal Investigator: Warren Washington, NCAR
7,500,000 processor hours, IBM Blue Gene/P, Argonne; 30,000,000 processor hours, Cray XTs, ORNL

"Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles"
Principal Investigator: Christopher Wolverton, Northwestern University
1,000,000 processor hours, IBM Blue Gene/P, Argonne

"First Principles Models of Type Ia Supernovae"
Principal Investigator: Stan Woosley, UCSC
3,000,000 processor hours, Cray XTs, ORNL

"Performance Evaluation and Analysis Consortium End Station"
Principal Investigator: Patrick H. Worley, ORNL
8,000,000 processor hours, IBM Blue Gene/P, Argonne; 8,000,000 processor hours, Cray XTs, ORNL

"Electronic, Lattice, and Mechanical Properties of Novel Nano-Structured Bulk Materials"
Principal Investigator: Jihui Yang, General Motors Research and Development Center
15,000,000 processor hours, Cray XTs, ORNL

2008 INCITE Awards

"Computational Protein Structure Prediction and Protein Design"
Principal Investigator: David Baker, University of Washington
12,000,000 processor hours, IBM Blue Gene/P, Argonne

"Interaction of Turbulence and Chemistry in Lean Premixed Laboratory Flames"
Principal Investigator: John Bell, LBNL
3,384,615 processor hours, NERSC HPC, NERSC

"The Role of Eddies in the Meridional Overturning Circulation"
Principal Investigator: Paola Cessi, UCSD
486,000 processor hours, Cray X1E, ORNL

"High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels"
Principal Investigator: Jacqueline Chen, Sandia
18,000,000 processor hours, Cray XT4, ORNL

"Computational Nuclear Structure"
Principal Investigator: David Dean, ORNL
10,000,000 processor hours, IBM Blue Gene/P, Argonne; 7,500,000 processor hours, Cray XT4, ORNL

"Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas"
Principal Investigator: Patrick Diamond, UCSD
8,000,000 processor hours, Cray XT4, ORNL

"Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence"
Principal Investigator: William Dorland, University of Maryland
4,000,000 processor hours, Cray XT4, ORNL

"Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows"
Principal Investigator: Hermann Fasel, University of Arizona
400,000 processor hours, Cray X1E, ORNL

"Large-Scale Simulations of Cardiac Electrical Activity"
Principal Investigator: Jeffrey Fox, Gene Network Sciences
846,720 processor hours, IBM Blue Gene/P, Argonne

"Modeling the Rheological Properties of Concrete"
Principal Investigator: William George, NIST
750,000 processor hours, IBM Blue Gene/P, Argonne

"An Integrated Approach to the Rational Design of Chemical Catalysts"
Principal Investigator: Robert Harrison, ORNL
10,000,000 processor hours, Cray XT4, ORNL

"Understanding the Electronic Structure of Novel Electronic Materials Using Many-Body Perturbation Theory"
Principal Investigator: Leeor Kronik, Weizmann Institute of Science
124,615 processor hours, NERSC HPC, NERSC

"Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models"
Principal Investigator: Don Lamb, ASC/Alliance Flash Center, University of Chicago
21,000,000 processor hours, IBM Blue Gene/P, Argonne

"Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling"
Principal Investigator: Lie-Quan Lee, Stanford Linear Accelerator Center
4,500,000 processor hours, Cray XT4, ORNL

"Multidimensional Simulations of Core Collapse Supernovae"
Principal Investigator: Anthony Mezzacappa, ORNL
16,000,000 processor hours, Cray XT4, ORNL

"BG/P Plan 9 Measurements on Large Scale Systems"
Principal Investigator: Ronald Minnich, Sandia
1,000,000 processor hours, IBM Blue Gene/P, Argonne

"Molecular Simulation of Complex Chemical Systems"
Principal Investigator: Christopher Mundy, PNNL
750,000 processor hours, IBM Blue Gene/P; 750,000 processor hours, Cray XT4, ORNL

"Modeling Heliospheric Phenomena with an Adaptive, MHD-Boltzmann Code"
Principal Investigator: Nikolai Pogorelov, University of California, Riverside
850,000 processor hours, Cray XT4, ORNL

"Massively Parallel Simulation of Combustion in Gas turbines"
Principal Investigator: Thierry Poinsot, CERFACS
4,000,000 processor hours, IBM Blue Gene/P, Argonne

"Beam Delivery System Optimization for X-Ray Free Electron Lasers"
Principal Investigator: Ji Qiang, LBNL
769,231 processor hours, NERSC HPC, NERSC

"Simulation of Global Cloudiness"
Principal Investigator: David Randall, Colorado State University
153,846 processor hours, NERSC HPC, NERSC

"Three-Dimensional Particle-in-Cell Simulations of Fast Ignition"
Principal Investigator: Chuang Ren, University of Rochester
307,692 processor hours, NERSC HPC, NERSC

"Predictive and Accurate Monte Carlo based simulations for Mott insulators, cuprate superconductors, and nanoscale systems."
Principal Investigator: Thomas Schulthess, ORNL
10,000,000 processor hours, Cray XT4, ORNL

"Predictions of Thermal Striping in Sodium Cooled Reactors"
Principal Investigator: Andrew Siegel, Argonne
5,000,000 processor hours, IBM Blue Gene/P, Argonne

"Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"
Principal Investigator: Jeremy Smith, ORNL
3,500,000 processor hours, Cray XT4, ORNL

"Lattice QCD"
Principal Investigator: Robert Sugar, University of California, Santa Barbara
19,600,000 processor hours, IBM Blue Gene/P, Argonne; 7,100,000 processor hours, Cray XT4, ORNL

"Clean and Efficient Coal Gasifier Designs Using Large-Scale Simulations"
Principal Investigator: Madhava Syamlal, National Energy Technology Laboratory
3,000,000 processor hours, Cray XT4, ORNL

"High Resolution Global Simulation of Plasma Microturbulence"
Principal Investigator: William Tang, PPPL
2,000,000 processor hours, IBM Blue Gene/P, Argonne

"Climate-Science Computational End Station Development and Grand Challenge Team"
Principal Investigator: Warren Washington, NCAR
1,000,000 processor hours, IBM Blue Gene/P, Argonne; 1,308,000 processor hours, NERSC HPC, NERSC; 15,718,000 processor hours, Cray XT4, ORNL

"Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles"
Principal Investigator: Christopher Wolverton, Northwestern University
1,000,000 processor hours, IBM Blue Gene/P, Argonne

"Electronic, Lattice, and Mechanical Properties of Novel Nano-Structured Bulk Materials"
Principal Investigator: Jihui Yang, GM R&D Center
10,000,000 processor hours, Cray XT4, ORNL

"Molecular Simulations of Surfactant Assisted Aqueous Foam Formation"
Principal Investigator: Kelly Anderson, Procter and Gamble and Pierre Verstraete, Procter and Gamble
4,000,000 processor hours, IBM Blue Gene/P, Argonne

"CAE Simulation of Full Vehicle Windnoise and Other CFD Phenomena"
Principal Investigator: Paul Bemis, Fluent Inc.
153,846 processor hours, NERSC HPC, NERSC

"High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability"
Principal Investigator: Peter Bradley, Pratt & Whitney
1,377,000 processor hours, IBM Blue Gene/P, Argonne

"Gyrokinetic Steady State Transport Simulations"
Principal Investigator: Jeff Candy, General Atomics
1,500,000 processor hours, Cray XT4, ORNL

"Numerical Relativity Simulations of Binary Black Holes and Gravitational Radiation"
Principal Investigator: Joan Centrella, NASA Goddard
1,000,000 processor hours, Cray XT4, ORNL

"Computational Rheology of Dense Suspensions"
Principal Investigator: Athonu Chatterjee, Corning Inc.
750,000 processor hours, HP-MPP, PNNL

"The 20th Century Reanalysis Project"
Principal Investigator: Gilbert Compo, University of Colorado Cooperative Institute for Research in the Environmental Sciences Climate Diagnostics Center and NOAA Earth System Research Laboratory
2,861,538 processor hours, NERSC HPC, NERSC

"Reactor Core Hydrodynamics"
Principal Investigator: Paul Fischer, Argonne
14,000,000 processor hours, IBM Blue Gene/P, Argonne

"Water in Confined States"
Principal Investigator: Giulia Galli, University of California, Davis
6,000,000 processor hours, IBM Blue Gene/P, Argonne

"Development and Correlations of Large Scale Computational Tools for Flight Vehicles"
Principal Investigator: Moeljo Hong, the Boeing Company
100,000 processor hours, Cray XT4, ORNL; 300,000 processor hours, Cray X1E, ORNL

"Direct Numerical Simulation of Turbulent Flame Quenching by Fine Water Droplets"
Principal Investigator: Hong Im, University of Michigan
307,692 processor hours, NERSC HPC, NERSC

"High Power Electromagnetic Wave Heating in the ITER Burning Plasma"
Principal Investigator: E. Fred Jaeger, ORNL
1,000,000 processor hours, Cray XT4, ORNL

"Modeling Reactive Flows in Porous Media"
Principal Investigator: Peter Lichtner, LANL
1,800,000 processor hours, Cray XT4, ORNL; 200,000 processor hours, HP-MPP, PNNL

"Assessing Global Climate Response of the NCAR-CCSM3: CO2 Sensitivity and Abrupt Climate Change"
Principal Investigator: Zhengyu Liu, University of Wisconsin - Madison
420,000 processor hours, Cray X1E, ORNL

"Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Principal Investigator: Warren Mori, UCLA
923,077 processor hours, NERSC HPC, NERSC

"Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean"
Principal Investigator: Synte Peacock, ASC/Alliance Flash Center, University of Chicago
3,163,000 processor hours, Cray XT4, ORNL

"Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences"
Principal Investigator: Michael Pindzola, Auburn University
2,000,000 processor hours, Cray X1E, ORNL

"Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates"
Principal Investigator: Lawrence Pratt, Fisk University
138,462 processor hours, NERSC HPC, NERSC

"Bose-Einstein Condensation vs. Quantum Localization in Quantum Magnets"
Principal Investigator: Tommaso Roscilde, Max-Planck Gesellschaft
1,200,000 processor hours, Cray XT4, ORNL

"Gating Mechanism of Membrane Proteins"
Principal Investigator: Benoit Roux, Argonne & the University of Chicago
1,500,000 processor hours, IBM Blue Gene/P, Argonne; 3,500,000 processor hours, Cray XT4, ORNL

"Simulation and Modeling of Synuclein-Based 'Protofibril Structures' as a Means of Understanding the Molecular Basis of Parkinson's Disease"
Principal Investigator: Igor Tsigelny, UCSD / SDSC
1,200,000 processor hours, IBM Blue Gene/P, Argonne

"Linear Scale Electronic Structure Calculations for Nanostructures"
Principal Investigator: Lin-Wang Wang, LBNL
2,100,000 processor hours, Cray XT4, ORNL

"First Principles Models of Type Ia Supernovae"
Principal Investigator: Stan Woosley, UCSC
3,500,000 processor hours, Cray XT4, ORNL

"Performance Evaluation and Analysis Consortium End Station"
Principal Investigator: Patrick H. Worley, ORNL
4,000,000 processor hours, IBM Blue Gene/P, Argonne; 4,000,000 processor hours, Cray XT4, ORNL

2007 INCITE Awards

"Molecular Simulations of Surfactant Assisted Aqueous Foam Formation"
Principal Investigator: Kelly Anderson, Procter and Gamble; Pierre Verstraete, Procter and Gamble
1,100,000 processor hours, IBM Blue Gene/L, Argonne

"CAE Simulation of Full Vehicle Wind Noise and Other CFD Phenomena"
Principal Investigator: Paul Bemis, Fluent Inc.
166,000 processor hours, NERSC HPC, NERSC

"Gyrokinetic Steady State Transport Simulations"
Principal Investigator: Jeff Candy, General Atomics
1,000,000 processor hours, Cray XT3, ORNL

"Numerical Relativity Simulations of Binary Black Holes and Gravitational Radiation"
Principal Investigator: Joan Centrella, NASA Goddard Space Flight Center
500,000 processor hours, Cray XT3, ORNL

"Computational Rheology of Dense Suspensions"
Principal Investigator: Athonu Chatterjee, Corning Incorporated
750,000 processor hours, HP-MPP, PNNL

"The 20th Century Reanalysis Project"
Principal Investigator: Gilbert Compo, University of Colorado Cooperative Institute for Research in the Environmental Sciences Climate Diagnostics Center and NOAA Earth System Research Laboratory
2,000,000 processor hours, NERSC HPC, NERSC

"Lattice QCD for Hadronic and Nuclear Physics"
Principal Investigator: Robert Edwards, Jefferson Laboratory
10,000,000 processor hours, Cray XT3, ORNL

"Reactor Core Hydrodynamics"
Principal Investigator: Paul Fischer, Argonne
1,000,000 processor hours, IBM Blue Gene/L, Argonne

"Water in Confined States"
Principal Investigator: Giulia Galli, University of California, Davis
1,500,000 processor hours, IBM Blue Gene/L, Argonne

"Direct Numerical Simulation of Turbulent Flame Quenching by Fine Water Droplets"
Principal Investigator: Hong Im, University of Michigan
1,000,000 processor hours, NERSC HPC, NERSC

"High Power Electromagnetic Wave Heating in the ITER Burning Plasma"
Principal Investigator: E. Fred Jaeger, ORNL
500,000 processor hours, Cray XT3, ORNL

"Study of the Gravitationally Confined Detonation Mechanism for Type Ia Supernovae"
Principal Investigator: Don Lamb, ASC/Alliance Flash Center, University of Chicago
Machine (Allocation): NERSC HPC (2,500,000 processor hours)

"Modeling Reactive Flows in Porous Media"
Principal Investigator: Peter Lichtner, LANL
Machine (Allocation): Cray XT3 (1,000,000 processor hours)

"Assessing Global Climate Response of the NCAR-CCSM3: CO2 Sensitivity and Abrupt Climate Change"
Principal Investigator: Zhengyu Liu, University of Wisconsin - Madison
420,000 processor hours, Cray X1E, ORNL

""Via Lactea': A Billion Particle Simulation of the Milky Way's Dark Matter Halo"
Principal Investigator: Piero Madau, UCSC
1,500,000 processor hours, Cray XT3, ORNL

"Ab Initio Modeling of the Glass Transition"
Principal Investigator: John Mauro, Corning Incorporated
100,000 processor hours, Cray X1E, ORNL

"Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Principal Investigator: Warren Mori, UCLA
1,000,000 processor hours, NERSC HPC, NERSC

"Statistical Physics of Fracture: Scientific Discovery through High-Performance Computing"
Principal Investigator: Phani Nukala, ORNL
1,100,000 processor hours, IBM Blue Gene/L, Argonne

"Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean"
Principal Investigator: Synte Peacock, ASC/Alliance Flash Center, University of Chicago
3,000,000 processor hours, Cray XT3, ORNL

"Three-Dimensional Particle-in-Cell Simulations for Fast Ignition"
Principal Investigator: Chuang Ren, University of Rochester
2,000,000 processor hours, NERSC HPC, NERSC

"Bose-Einstein Condensation vs. Quantum Localization in Quantum Magnets"
Principal Investigator: Tommaso Roscilde, Max-Planck Gesellschaft
800,000 processor hours, Cray XT3, ORNL

"Gating Mechanism of Membrane Proteins"
Principal Investigator: Benoit Roux, Argonne and the University of Chicago
4,000,000 processor hours, Cray XT3, ORNL

"Coherent Control of Light in Nanoscale"
Principal Investigator: Tamar Seideman, Northwestern University
600,000 processor hours, IBM Blue Gene/L, Argonne

"Linear Scale Electronic Structure Calculations for Nanostructures"
Principal Investigator: Lin-Wang Wang, LBNL
1,500,000 processor hours, Cray XT3, ORNL

"First Principles Models of Type Ia Supernovae"
Principal Investigator: Stan Woosley, UCSC
4,000,000 processor hours, Cray XT3, ORNL

"Performance Evaluation and Analysis Consortium End Station"
Principal Investigator: Patrick H. Worley, ORNL
1,000,000 processor hours, Cray XT3, ORNL

"Next Generation Simulations in Biology: Investigating Iomolecular Structure, Dynamics and Function through Multi-Scale Modeling"
Principal Investigator: Pratul Agarwal, ORNL
1,000,000 processor hours, Cray XT3, ORNL

"High-Resolution Protein Struction Prediction"
Principal Investigator: David Baker, University of Washington / Howard Hughes Medical Institute
3,000,000 processor hours, IBM Blue Gene/L, Argonne

"Simulation of Wave-Plasma Interaction and Extended MHD in Fusion Systems"
Principal Investigator: Donald Batchelor, ORNL
2,000,000 processor hours, Cray XT3, ORNL

"High Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability"
Principal Investigator: Peter Bradley, Pratt & Whitney
750,000 processor hours, IBM Blue Gene/L, Argonne

"High-Fidelity Numerical Simulations of Turbulent Combustion—Fundamental Science towards Predictive Models"
Principal Investigator: Jackie Chen, Sandia
50,000 processor hours, Cray X1E, ORNL; 6,000,000 processor hours, Cray XT3, ORNL

"Ab Initio Nuclear Structure Computations"
Principal Investigator: David Dean, ORNL
5,000,000 processor hours, Cray XT3, ORNL

"An Integrated Approach to the Rational Design of Chemical Catalysts"
Principal Investigator: Robert Harrison, ORNL
300,000 processor hours, Cray X1E, ORNL; 3,000,000 processor hours, Cray XT3, ORNL

"Development and Correlations of Large Scale Computational Tools for Flight Vehicles"
Principal Investigator: Moeljo Hong, Boeing Company
200,000 processor hours, Cray X1E, ORNL

"Computational Design of the Low-loss Accelerating Cavity for the ILC"
Principal Investigator: Kwok Ko, Stanford Linear Accelerator Center
400,000 processor hours, Cray X1E, ORNL

"Gyrokinetic Plasma Simulation"
Principal Investigator: W.W. Lee, PPPL
75,000 processor hours, Cray X1E, ORNL; 6,000,000 processor hours, Cray XT3, ORNL

"Modeling the Response of Terrestrial Ecosystems to Climate Change and Disturbance"
Principal Investigator: David McGuire, University of Alaska, Fairbanks
600,000 processor hours, IBM Blue Gene/L, Argonne

"Multi-Dimensional Simulations of Core-Collapse Supernovae"
Principal Investigator: Anthony Mezzacappa, ORNL
300,000 processor hours, Cray X1E, ORNL; 7,000,000 processor hours, Cray XT3, ORNL

"Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences"
Principal Investigator: Michael Pindzola, Auburn University
750,000 processor hours, Cray X1E, ORNL

"Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates"
Principal Investigator: Lawrence Pratt, Fisk University
150,000 processor hours, NERSC HPC, NERSC

"Predictive Simulations in Strongly Correlated Electron Systems and Functional Nanostructures"
Principal Investigator: Thomas Schulthess, ORNL
500,000 processor hours, Cray X1E, ORNL; 7,000,000 processor hours, Cray XT3, ORNL

"Real-Time Ray-Tracing"
Principal Investigator: Evan Smyth, Dreamworks Animation
900,000 processor hours, Cray XT3, ORNL

"Simulation and Modeling of Synuclein-Based Protofibril Structures as a Means of Understanding the Molecular Basis of Parkinson's Disease"
Principal Investigator: Igor Tsigelny, UCSD / SDSC
75,000 processor hours, IBM Blue Gene/L, Argonne

"Interaction of ITG/TEM and ETG Gyrokinetic Turbulence"
Principal Investigator: Ronald Waltz, General Atomics
500,000 processor hours, Cray X1E, ORNL

"Climate-Science Computational End Station Development and Grand Challenge Team"
Principal Investigator: Warren Washington, NCAR
1,500,000 processor hours, Cray X1E, ORNL; 4,000,000 processor hours, Cray XT3, ORNL

2006 INCITE Awards

"Development and Correlations of Large Scale Computational Tools for Flight Vehicles"
Principal Investigator: Moeljo Hong, The Boeing Company
200,000 processor hours,Cray X1E, ORNL

"Interaction of ITG/TEM and ETG gyrokinetic turbulence"
Principal Investigator: Ronald Waltz, General Atomics
400,000 processor hours, Cray X1E, ORNL

"Molecular Dynamics of Molecular Motors"
Principal Investigator: Martin Karplus, Harvard University
1,484,800 processor hours, Cray XT3, ORNL

"Real-Time Ray-Tracing"
Principal Investigator: Evan Smyth, Dreamworks Animation
950,000 processor hours, Cray XT3, ORNL

"Direct Numerical Simluation of Fracture, Fragmentation and Localization in Brittle and Ductile Materials"
Principal Investigator: Michael Ortiz, California Institute of Technology
500,000 processor hours, Cray XT3, ORNL

"Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences"
Principal Investigator: Michael Pindzola, Auburn University
650,000 processor hours, HP-MPP, PNNL

"High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability"
Principal Investigator: Robert Malecki, Pratt & Whitney
888,400 processor hours, IBM Blue Gene, Argonne

"Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture"
Principal Investigator: Phani Nukala, ORNL
1,500,000 processor hours, IBM Blue Gene, Argonne

"Modeling the Response of Terrestrial Ecosystems to Climate Change and Disturbance"
Principal Investigator: David McGuire, University of Alaska, Fairbanks
600,000 processor hours, IBM Blue Gene, Argonne

"Computational Spectroscopy of Aqueous Solutions"
Principal Investigator: Giulia Galli, University of California, Davis
2,500,000 processor hours, IBM Blue Gene, Argonne

"High Resolution Protein Structure Prediction"
Principal Investigator: David Baker, University of Washington/ Howard Hughes Medical Institute
5,000,000 processor hours, IBM Blue Gene, Argonne

"High Resolution Protein Structure Prediction"
Principal Investigator: David Baker, University of Washington/ Howard Hughes Medical Institute
5,000,000 processor hours, IBM Blue Gene, Argonne

"Simulation and Modeling of Synuclein-Based 'Protofibril Structures' as a Means of Understanding the Molecular Basis of Parkinson's Disease"
Principal Investigator: Igor Tsigelny, UCSD / SDSC
16,000 processor hours, IBM Blue Gene, Argonne

"Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates"
Principal Investigator: Lawrence Pratt, Fisk University
50,000 processor hours, IBM Blue Gene, Argonne

"Precision Cosmology Using Lyman Alpha Forest"
Principal Investigator: Michael Norman, UCSD
1,000,000 processor hours, IBM Power 3+, NERSC

"Particle in Cell Simulation of Laser Wakefield Particle Acceleration"
Principal Investigator: Cameron Geddes, LBNL
2,500,000 processor hours, IBM Power 3+, NERSC

2005 INCITE Awards

"Magneto-Rotational Instability and Turbulent Angular Momentum Transport"
Principal Investigator: Fausto Cattaneo, University of Chicago
2,000,000 processor hours, IBM SP, NERSC

"Direct Numerical Simulation of Turbulent Non-Premixed Combustion—Fundamental Insights towards Predictive Modeling"
Principal Investigator: Jacqueline Chen and Evatt Hawkes, Sandia
2,500,000 processor hours, IBM SP, NERSC

"Molecular Dynamics"
Principal Investigator: Valerie Dagget, University of Washington
2,000,000 processor hours, IBM SP, NERSC

2004 INCITE Awards

"Thermonuclear Supernovae: Stellar Explosions in Three Dimensions"
Principal Investigator: Tomasz Plewa, Center for Astrophysical Thermonuclear Flashes, University of Chicago
2,700,000 processor hours, IBM SP, NERSC

"Fluid Turbulence and Mixing at High Reynolds Number"
Principal Investigator: P.K. Yeung, Georgia Institute of Technology
1,200,000 processor hours, IBM SP, NERSC

"Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers"
Principal Investigator: William A. Lester, Jr, LBNL and the University of California-Berkeley
1,000,000 processor hours, IBM SP, NERSC

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