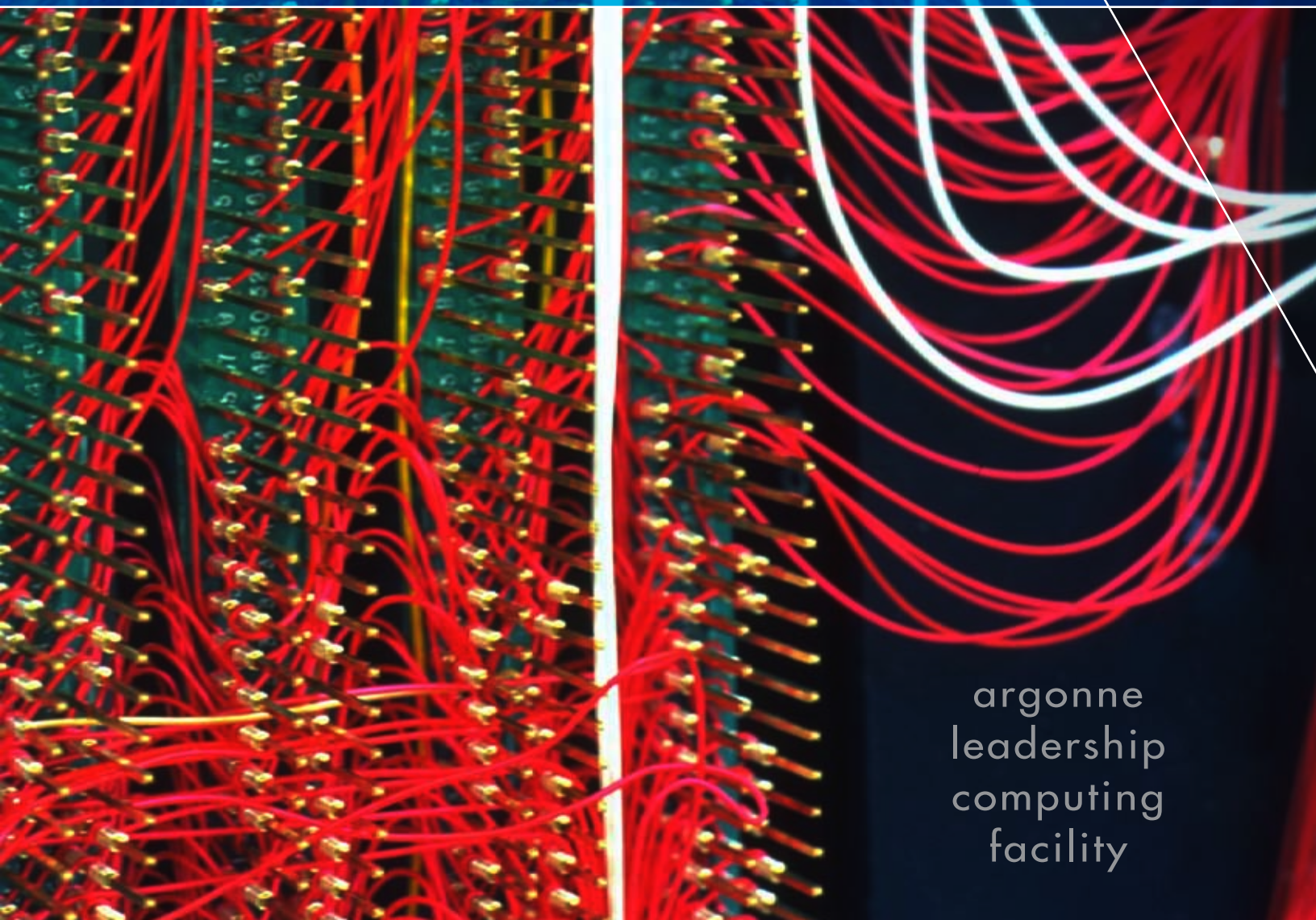
argonne leadership computing facility

dedicated to breakthrough science and engineering

Argonne NATIONAL LABORATORY

Accelerating Scientific Discovery

2007 Annual Report



argonne leadership computing facility

The Argonne Leadership Computing Facility team provides expert assistance and support to researchers in maximizing the impact of supercomputing capabilities on scientific discovery.

contents

accelerating scientific discovery

welcome

Dr. Peter Beckman
ALCF Acting Division Director

As a gateway for scientific discovery, the Argonne Leadership Computing Facility (ALCF) works hand in hand with the world's best computational scientists to advance research in a diverse span of scientific domains, ranging from chemistry, applied mathematics, and materials science to engineering physics and life sciences.

Sponsored by the U.S. Department of Energy's (DOE) Office of Science, researchers are using the IBM Blue Gene/L supercomputer at the ALCF to study and explore key scientific problems that underlie important challenges facing our society (see page 5). For instance, a research team at the University of California-San Diego/SDSC is studying the molecular basis of Parkinson's disease. The researchers plan to use the knowledge they gain to discover new drugs to treat the disease and to identify risk factors for other diseases that are equally prevalent. Likewise, scientists from Pratt & Whitney are using the Blue Gene to understand the complex processes within aircraft engines. Expanding our understanding of jet engine combustors is the secret to improved fuel efficiency and reduced emissions. Lessons learned from the scientific simulations of jet engine combustors have already led Pratt & Whitney to newer designs with unprecedented reductions in emissions, noise, and cost of ownership.

ALCF staff members provide in-depth expertise and assistance to those using the Blue Gene/L and optimizing user applications. Both the Catalyst and Applications Performance Engineering and Data Analytics (APEDA) teams support the users' projects.

In addition to working with scientists running experiments on the Blue Gene/L, we have become a nexus for the broader global community. In partnership with the Mathematics and Computer Science Division at Argonne National Laboratory, we have created an environment where the world's most challenging computational science problems can be addressed. Our expertise in high-end scientific computing enables us to provide guidance for applications that are transitioning to petascale as well as to produce software that facilitates their development, such as the MPICH library, which provides a portable and efficient implementation of the MPI standard—the prevalent programming model for large-scale scientific applications—and the PETSc toolkit that provides a programming paradigm that eases the development of many scientific applications on high-end computers.

I would especially like to thank our user community, whose achievements we are showcasing here. They are our most important partners as we boldly seek to solve today's most pressing computational science problems and progress toward exascale computational science tomorrow.

DOE's INCITE program

Over the past 30 years, the U.S. Department of Energy's (DOE) high-performance computing program has played an increasingly important role in scientific research by allowing scientists to create more accurate models of processes, simulate problems that were once thought impossible, and analyze the increasing amount of data generated by experiments.

DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program builds on this tradition. Launched in 2003, INCITE annually awards researchers millions of supercomputer processor hours and 100 trillion bytes of data storage space at DOE's global flagship facilities for unclassified supercomputing. These facilities, including the Argonne Leadership Computing Facility (ALCF), house some of the most powerful computers in the world. Detailed descriptions of the systems can be found on DOE's Office of Science website.

The INCITE program seeks computationally intensive, large-scale research projects that can make high-impact scientific advances through the use of this substantial allocation of computer time and data storage. The program encourages proposals from universities, research institutions, and industry. Industry is specifically solicited to propose challenging problems that may be solved using high-performance computing. Proposals are peer reviewed and are chosen solely on the basis of scientific merit.

In 2007, INCITE awarded 9 research projects nearly 10 million hours of computing time on IBM Blue Gene/L supercomputers at the ALCF and the IBM T. J. Watson Research Center. The projects are listed in the accompanying sidebar and highlighted in more detail on pp. 7-23 of this report.

INCITE has produced significant accomplishments. Through INCITE, scientists studying supernovae were able to model the first-ever full-star simulations of stellar explosions in three dimensions. Another group used their INCITE allocation to study key aspects of photosynthesis to better understand this sustainable energy source. A third group was able to create simulations of turbulence at a scale of unsurpassed detail, which can be used to improve engineering processes.

The program continues to grow at a rapid pace and promises to deliver breakthrough science and engineering that will address the world's toughest challenges for decades to come.

2007 INCITE Projects at the ALCF

- High-Resolution Protein Structure Prediction *(University of Washington/ Howard Hughes Medical Institute)*
- Reactor Core Hydrodynamics *(Argonne National Laboratory, University of Illinois)*
- High-Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability *(Pratt & Whitney)*
- Molecular Simulations of Surfactant-Assisted Aqueous Foam Formation *(Procter & Gamble, University of Pennsylvania)*
- Coherent Control of Light in Nanoscale *(Northwestern University)*
- Water in Confined States *(University of California-Davis, Lawrence Livermore National Laboratory)*
- Simulation and Modeling of Synuclein-Based Protofibril Structures As a Means of Understanding the Molecular Basis of Parkinson's Disease *(University of California-San Diego/ SDSC)*
- Statistical Physics of Fracture: Scientific Discovery through High-Performance Computing *(Oak Ridge National Laboratory)*
- Modeling the Response of Terrestrial Ecosystems to Climate Change and Disturbance *(University of Alaska, Fairbanks)*

overview

ALCF Accelerates Scientific Discovery

In 2007, scientists tackled some of the world's most complex computational challenges on the IBM Blue Gene/L supercomputer at the Argonne Leadership Computing Facility (ALCF). The 2,048-processor, 5.7 teraflops Blue Gene/L rapidly accelerated the pace of scientific discovery in a wide array of disciplines, including biology, life sciences, chemical sciences, physical chemistry, materials sciences, and engineering physics.

ALCF Mission

The ALCF is a U.S. Department of Energy (DOE) national leadership-class computing facility sponsored by DOE's Office of Advanced Scientific Computing Research, Office of Science. Its mission is to provide the computational science community with a leading computing capability dedicated to breakthrough science and engineering.

ALCF Vision

The ALCF strives to be the forefront computational center for extending the frontiers of science by solving important problems for the nation that require innovative approaches and the largest-scale systems to solve.

ALCF Achievements

The ALCF made significant progress during 2007 in meeting key objectives and establishing core capabilities to fulfill its long-term mission. Major milestones were reached in scientific impact, facility build-out, organizational expansion, operations, and outreach.

Through a variety of outreach activities, such as workshops, exhibits, and a job fair, ALCF staff kept INCITE researchers, supercomputing colleagues, and students well informed throughout the year.

"We're pleased to see such a wide range of projects being run on Blue Gene. The diversity of this research is a testament to the enduring utility of the Blue Gene design and offers a glimpse of the commercial potential that is the future of supercomputing."

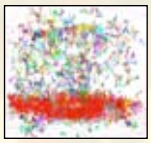
David Turek
Vice President of IBM's Deep Computing Group

The ALCF's 2007 INCITE projects encompassed the following research endeavors:

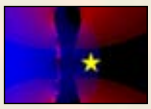
- Kelly Anderson at Procter & Gamble investigated the molecular mechanisms of bubble formation in foams to help develop better fire control chemicals and environmentally friendly consumer products.

- Giulia Galli at the University of California–Davis, in collaboration with Lawrence Livermore National Laboratory, simulated water in confined spaces to study water flow and transport at the nanoscale relevant to both materials science and biological problems.

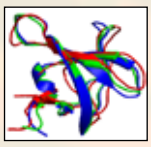
- Paul Fischer at Argonne National Laboratory, with collaborators at the University of Illinois, studied turbulent thermal transport in sodium-cooled reactor cores in order to gain an understanding of thermal mixing that can lead to improved safety and economy of advanced reactors.



- Phani Nukala at Oak Ridge National Laboratory simulated the physics of fracture that may resolve controversies about how the presence and distribution of disorder impacts materials fracture propagation and related properties.



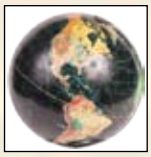
- Tamar Seideman at Northwestern University modeled the manipulation of light at the nanoscale, with potential applications in solar energy, sensors, and chemistry.



- David Baker at the University of Washington undertook the high-resolution prediction of protein structures with up to 150 amino acids in protein families that have unknown structures to aid in understanding their functions.

- Peter Bradley at Pratt & Whitney conducted high-fidelity simulations of an aircraft engine combustor that properly resolve turbulence, thereby improving emissions and operability of future designs.

- Igor Tsigelny at the University of California–San Diego combined models of synuclein-based protofibril structures with experimental findings as a means of understanding the molecular basis of Parkinson's disease and generating leads for drug discovery.



- David McGuire at the University of Alaska–Fairbanks modeled the response of terrestrial ecosystems to climate change and disturbance to understand the changing cycles of carbon release in the higher latitudes.

ALCF staff members provided in-depth expertise and assistance to scientists using the BG/L and helped optimize user applications.

Timeline

2004

– Formed the Blue Gene Consortium with IBM

2005

– Installed 5-teraflops Blue Gene/L for evaluation

2006

– Began production support of 6 INCITE projects

– Continued code development and evaluation

2007

– Increased to 9 INCITE projects

– Continued development projects

– Held Next Generation Blue Gene workshop (June)

– Installed 100-teraflops Blue Gene/P (Oct.-Nov.)

– Accepted 100-teraflops Blue Gene/P (Dec.)

biology

ROSETTA Method Predicts Protein Structure

Researchers

David Baker
University of Washington/
Howard Hughes Medical Institute

Over the past several years, a research group at the University of Washington has developed and is now using the ROSETTA methodology for predicting computationally the structure of proteins—the workhorse molecules of all biological systems.

The goal is to create detailed, three-dimensional models of the structure of selected proteins at atomic-level resolution. Because the structure of a protein determines its function, this work will have an important impact on the prediction of how proteins connect or "dock" with each other and the actual design of proteins and drugs.

Under the DOE INCITE program, the research team worked to refine and expand the capabilities of the ROSETTA method by using the Blue Gene/L computers at the Argonne Leadership Computing Facility and the IBM T.J. Watson Research Center.

Scientific Approach

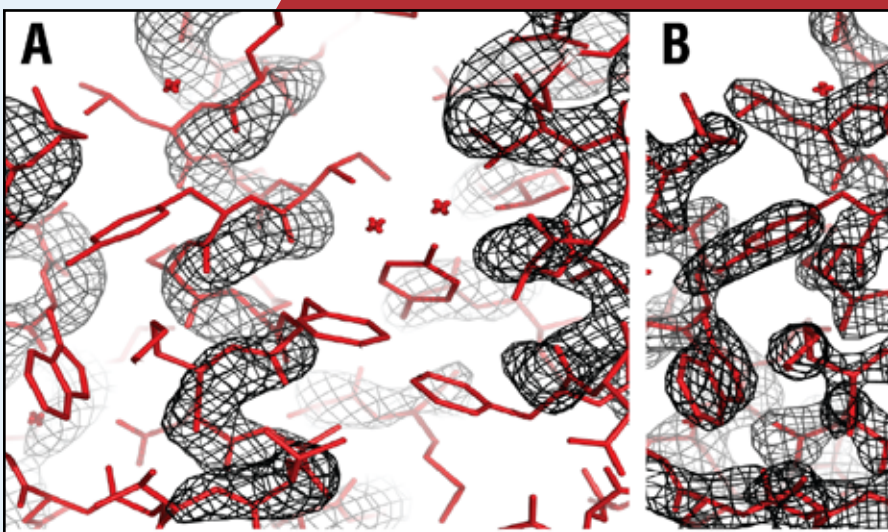
The ROSETTA method uses a two-phase Monte Carlo algorithm to sample the extremely large space of possible protein structures to find the most favorable one.

The first phase generates a low-resolution model of the protein backbone and approximates side chains with a single dummy atom. The high-resolution phase then uses a more realistic model of the full protein, along with corresponding information about interactions, to find the best candidate for the native structure.

A key application of the ROSETTA method is in refining homology models or low-resolution models obtained from limited Nuclear Magnetic Resonance (NMR) data. ROSETTA-refined models have proved sufficiently accurate to be suitable for molecular replacement solutions used in phasing X-ray crystallography data.

"The INCITE program has been critical to the progress made in protein structure modeling using ROSETTA."

David Baker
University of Washington
Department of Biochemistry



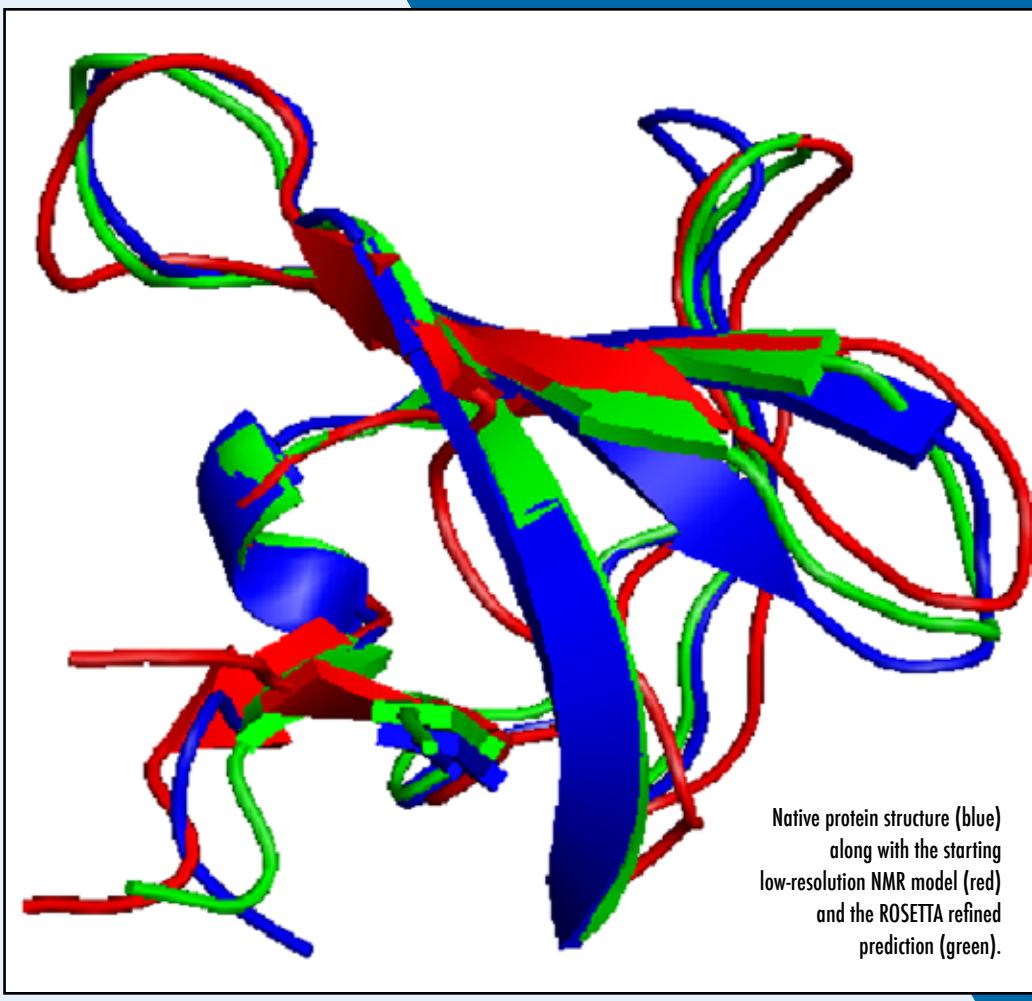
Research Results

Researchers have developed an all-atom protocol that can provide the full atomic-level structure of proteins. This new protocol has successfully predicted protein structure to atomic-level accuracy in a community-wide test.

The protocol uses a physically realistic high-resolution energy function that had been previously used in designing a novel protein fold with atomic-level accuracy.

Formerly, the ROSETTA method had been tested on several proteins of known structure having up to 189 amino acids. In many cases, the accuracy of the prediction was within a remarkable one angstrom of the experimentally solved high-resolution crystal structure.

Currently, the ROSETTA method is being tested on proteins of known structure to determine the size range and fold classes for which accurate results can be predicted.

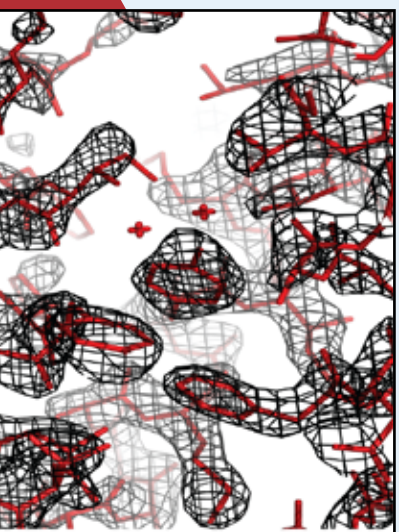


Native protein structure (blue) along with the starting low-resolution NMR model (red) and the ROSETTA refined prediction (green).

Looking Ahead

In future research, the ROSETTA method will be used to make predictions for proteins with unknown structures. One set of protein domains of interest consists of several hundred functionally annotated proteins in the human genome for which either (a) no structural information is available or (b) only structures of remote sequence homologues are available.

Also, efforts are under way to develop a high-throughput pipeline for predicting protein structures using sparse experimental data.



A picture of the electron density (black) generated from phases determined from the starting low-resolution NMR model (Panel A) and that generated from phases determined from the ROSETTA refined model (Panel B). The crystal structure (red) agrees very well with the phases determined from the ROSETTA model.

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reactor core hydrodynamics

Sodium-Cooled Fast Reactors Offer Economical Power, Nuclear Fuel Recyling

Researchers

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Carlos Pantano
University of Illinois

Andrew Siegel
Argonne National Laboratory

A new generation of sodium-cooled fast reactors proposes to close the fuel cycle by transmuting and reusing spent fuel from thermal reactors in advanced recycling reactors. Among the benefits would be an economically viable approach to significantly reduced loading (nearly a hundred-fold) in geological repositories. This Department of Energy (DOE) INCITE project focuses on two fundamental design issues for the sodium coolant flow, namely, pressure loss (or required pumping power) and the degree of cross-assembly mixing induced by wire wrap spacers that separate fuel pins within each subassembly.

Scientific Approach

These issues are being addressed through large eddy simulations (LES) of turbulent flow in a sequence of subassembly geometries. Direct numerical simulation of this flow is infeasible because of the range of spatial and temporal scales at Reynolds number Re~50,000, the non-dimensional velocity characteristic of the coolant flow. Fortunately, important macroscopic features of the flow are accessible by simulating only the larger eddies in the flow field, which allows a significant reduction in the number of grid points and timesteps required to represent the numerical solution. Even so, the large number of coolant passages at design scales necessitates petascale computing resources for a full subassembly of 217 pins. Consequently, researchers undertook a systematic approach involving a sequence of pin counts (1, 7, 19, 37, etc.), which allowed them to identify and decouple the important effects of side and corner channels from the predominant interior channels. Interior channel effects were isolated by simulating a single pin in a periodic array.

2007 INCITE simulations employed the 2,048-processor IBM Blue Gene/L at the Argonne Leadership Computing Facility. The computations were based on Nek5000, which simulates fluid flow, convective heat and species transport, and magneto-hydrodynamics in general 2-D and 3-D domains. Nek5000 was developed at Argonne National Laboratory under DOE's Advanced Scientific Computing Research program. A singular feature is the code's ability to scale to the large processor counts that characterize petascale computing platforms. Several features of Nek5000 make it highly suitable for petascale science. The spectral element (SE) method, on which the code is based, yields rapid numerical convergence, which implies that transport of small scale features over long times and distances incur minimal numerical dissipation and dispersion. In effect, accuracy per gridpoint is maximized. The code also features scalable multigrid methods capable of solving systems with 10^8 degrees of freedom in only 10-50 iterations.

2007 INCITE computations focused on a single pin in a periodic array and on the 7-pin case, which is the smallest configuration that features all three subchannel types. A cutaway view of the turbulent velocity field in a 7-pin configuration appears on page 11. The computational mesh of ~44 M gridpoints uses 132,000 elements of order N=7 (512 points per element).

"Advanced simulations are paving the way to application of petascale computing for reactor thermal hydraulics analysis and design."

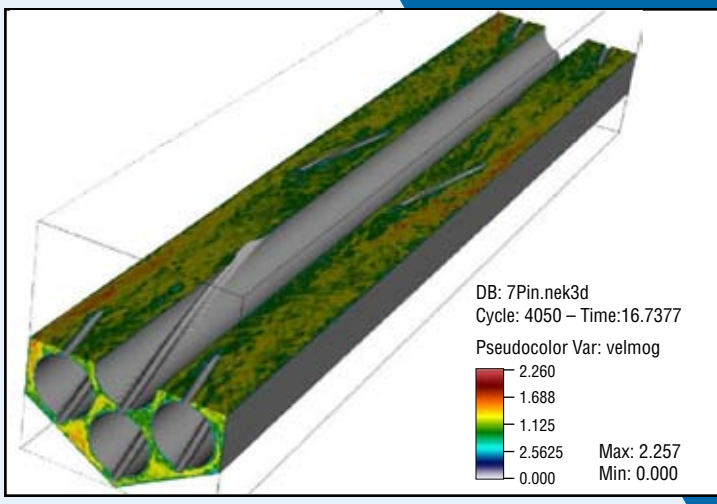
Paul Fischer
Argonne National Laboratory

Research Results

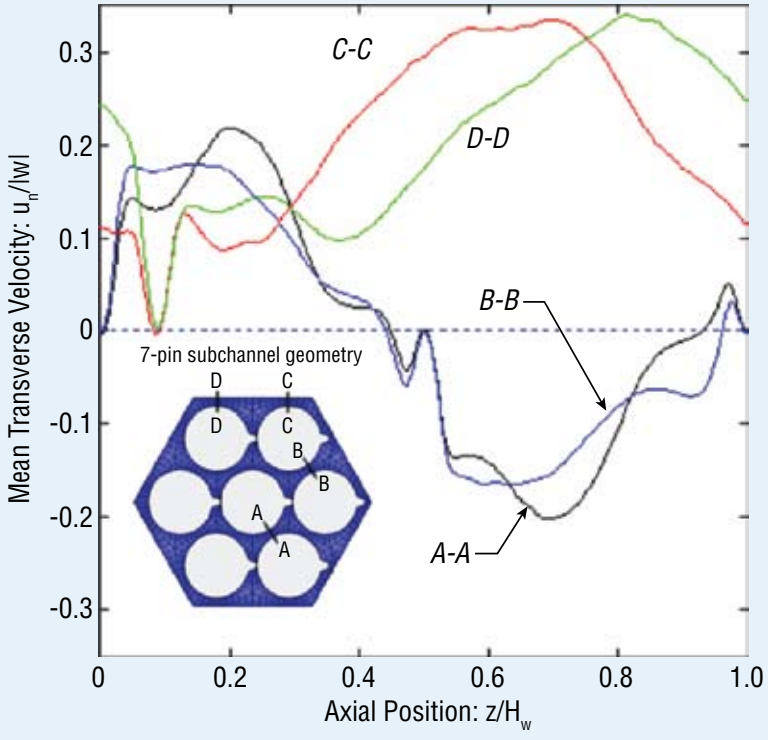
The single- and 7-pin simulations identified cross-flow velocities between coolant subchannels. These distributions are one of the key results from experiments and now simulations because they characterize the essential aspects of the velocity fields for subsequent design scoping studies. While the single-pin results exhibited a nearly sinusoidal cross-flow distribution as a function of axial position, the 7-pin results showed markedly different behavior. The interior distributions had higher wavenumber content and lower amplitude than the single-pin case. The exterior interfaces had nonzero means, which indicate a net swirling flow around the subassembly, as reported in previous experiments.

Looking Ahead

In addition to the results achieved, researchers quantified the effects of varying wire-wrap pitch for the single pin case and are now studying the same question for 7 pins. 19- and 37-pin configurations will be studied in 2008.



Turbulent velocity field in a 7-pin bundle with wire-wrap spacers.



7-pin cross flow distributions.

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engineering physics

P&W Improves Aircraft Engine Combustor Simulations

Researchers

Peter Bradley
Pratt & Whitney

A jet engine combustor combines air flowing faster than a hurricane with swirling fuel to generate the extraordinary release of heat that ultimately powers the aircraft. Understanding these complex physical and chemical interactions is critical to fuel efficiency and emissions performance, but physical testing can be difficult and time consuming. "Virtual Testing" with Computational Fluid Dynamics (CFD), the numerical simulation of fluid flows, can offer insights that are difficult to achieve with physical methods. However, industrial use of CFD for combustors is challenged by the inherent tradeoff between simulation fidelity and turnaround time.

Scientific Approach

Pratt & Whitney has been exploring leading-edge combustor design methods at the ALCF using the IBM Blue Gene supercomputer as part of the U.S. Department of Energy (DOE) INCITE program. This work is studying the effect of different fidelities of analysis as well as computational methods to reduce turnaround time. The goal is to define a design process that makes simulations that were traditionally challenging "one offs" usable in the production design cycle for next generation commercial and military jet engines.

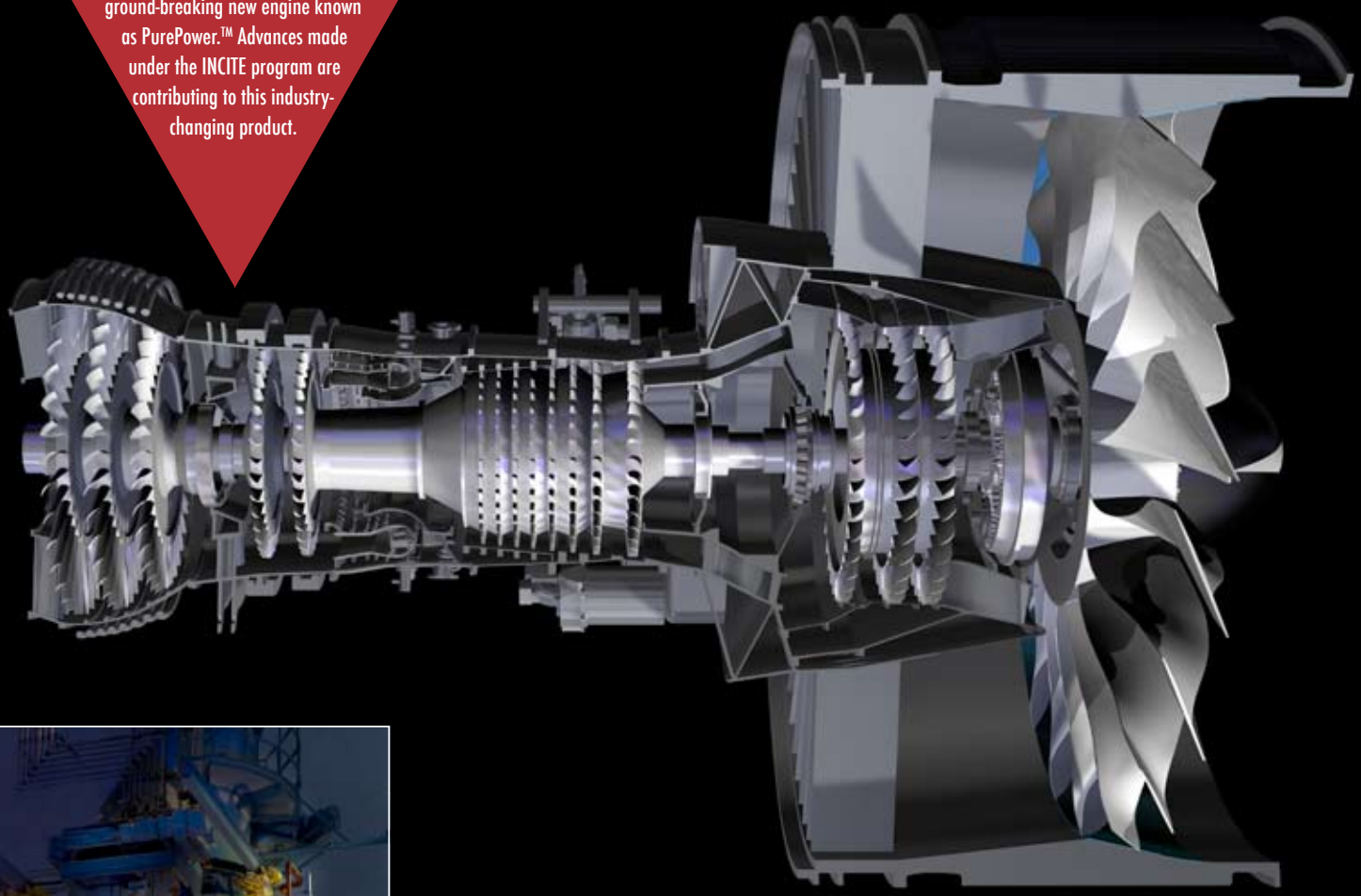
Research Results

This INCITE project has led to improved capabilities and reduced solution times for three-dimensional (3-D) combustor simulations. The work has been a key enabler for the depth of understanding needed to meet emissions goals. Capabilities improved through INCITE are now being applied to Pratt & Whitney's next-generation, low-emission PurePower™ engine. This groundbreaking engine will deliver unprecedented reductions in emissions, noise, and cost of ownership as compared to current engines.

"In an ever-expanding global economy where technology leadership is critical to competitiveness, INCITE provides American industry with an engine for technological and competitive growth."

Peter Bradley
Pratt & Whitney

Pratt & Whitney is developing a ground-breaking new engine known as PurePower.™ Advances made under the INCITE program are contributing to this industry-changing product.



PurePower™ will deliver double-digit reductions in fuel consumption, emissions, and cost of ownership.

Looking Ahead

Computing technology changes rapidly and compute power grows exponentially. This is an opportunity because it enables new analysis that can lead to improved products, but also a challenge as industry must leverage emerging opportunities to remain competitive. The ALCF gives industry early access to next-generation capabilities, which will improve competitiveness and enable advances that impact the lives of people throughout the world.

Researchers plan to use the Blue Gene's capabilities to complete high-fidelity simulations that will give new insights on aerodynamic behavior inside an operating jet engine combustor.

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chemical sciences

Virtual R&D, HPC Enable Breakthrough Innovation at P&G

Researchers

Kelly Anderson
Procter & Gamble

Michael Klein
University of Pennsylvania

Peter Koenig
Procter & Gamble

Tom Lange
Procter & Gamble

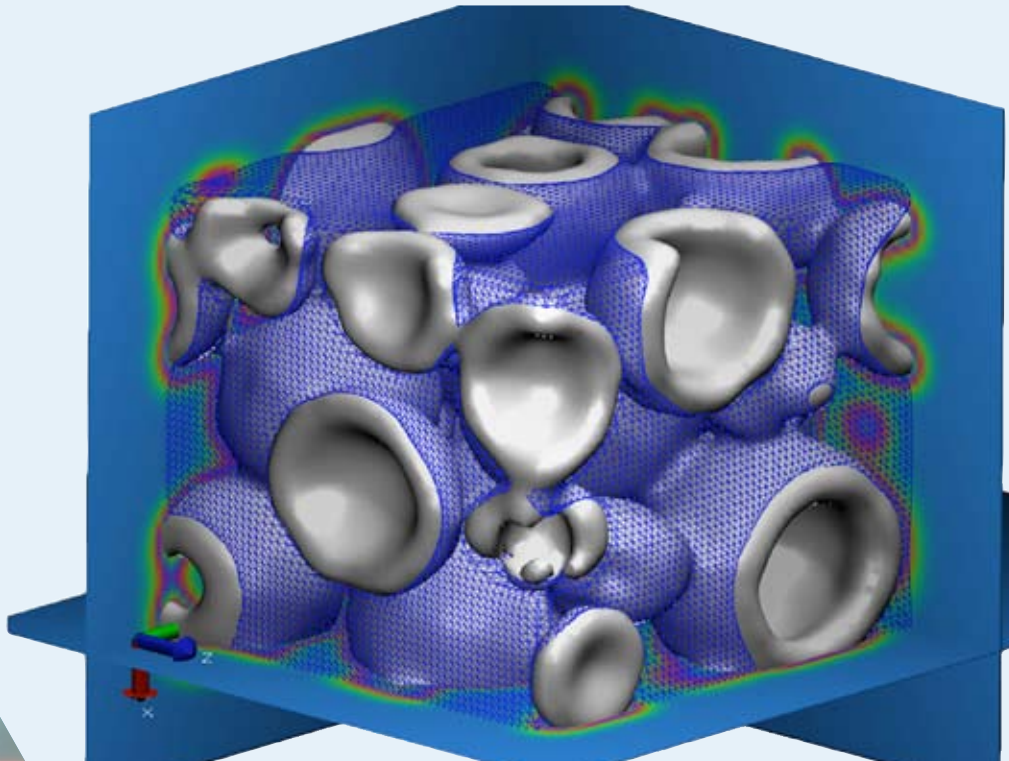
Some of the world's most well-known and highly regarded industrial companies have sought out Argonne's computing capacity and technical expertise to convert that knowledge into transformative products and technologies. In 2007, Procter & Gamble (P&G), one of the 25 largest U.S. companies by revenue, was awarded over one million processor-hours on Argonne's IBM Blue Gene/L supercomputer through the DOE INCITE program.

Virtual R&D and high performance computing play a significant role in P&G's R&D strategy and execution, ensuring that the company's innovations make it to the marketplace in a timely and cost-effective manner. P&G has significantly expanded capabilities in computational modeling and computer-aided engineering so the company can do an increasing percentage of product and process design through virtual simulation. Virtual prototyping gives researchers the ability to ask "what if," and then test the concept or product in any number of ways to determine next steps, if any, moving forward.

Scientific Approach

Some of P&G's longer-term scientific and engineering investigations are being pursued through modeling and simulation technology at a scale previously thought impossible.

P&G researchers used the Blue Gene/L system at the Argonne Leadership Computing Facility (ALCF) to investigate the molecular mechanisms of bubble formation in foams. Until recently, most knowledge of how suds form and break down was based primarily on experience and observation. However, an understanding of these processes is critical in the development of many consumer goods, foods, and fire control materials. Through its collaboration with the ALCF, P&G utilized LAMMPS, a DOE code.



"This grant allows us to perform computer simulations, at an unprecedented scale, on the dissolving of soap and forming of suds. The resulting approach should help us formulate products faster and more efficiently. That means the consumer wins by getting better products sooner, and at better value, than would have been possible using traditional methods."

Kelly Anderson
Procter & Gamble

Research Results

Researchers have observed the early stages of bubble formation in full atomistic detail, allowing them to directly observe the lowering of surface tension as a function of molecular composition and time. They also have demonstrated the "Marongoni effect" at the atomistic level. These data are used to generate accurate coarse-grained molecular simulation parameters, which will then be used to study even larger simulation domains.

Looking Ahead

Future work in this area will extend existing coarse-grained force fields to enable studies of even more diverse ionic surfactants and polymers at the air-water interface. Using dynamic simulations, researchers will show the relationship between molecular structure and the kinetics of foam formation. Given success, the model will be extended to investigate the role of polymers in foam stabilization, and P&G will continue to work with the University of Pennsylvania to advance simulation methods and material understanding.

This image represents a 3-D periodic mesoscale simulation of many small bubbles that exist during the early stages of foam formation. Results show that by using different surfactant structures, different bubble profiles can be produced. The blue mesh represents water, while surfactant molecules are represented by the white isosurfaces. VMD was used to create this visualization.

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physical chemistry

Northwestern Researchers Explore Coherent Control of Light in Nanoscale Devices

Researchers

Tamar Seideman
Northwestern University

Maxim Sukharev
Northwestern University

Researchers at Northwestern University are working to understand, model, and manipulate light propagation in the nanoscale realm, where dimensions are measured in billionths of a meter. In particular, they are exploring the control of light (photons) using ultra-small metal particles and their arrays, and developing a new approach to the design of nanoscale devices with desired functionalities.

Nanophotonic concepts are already being applied in novel sensors, medical diagnostic systems, nonlinear light sources, and various spectroscopies. In the future, researchers expect these concepts to also make possible subdiffraction waveguides, control of chemical processes at the nanoscale, and new nanoscale probes.

Although experimentally one can size, shape, and arrange particles with precision, a crucial question is how to structure them so as to achieve a desired optical property or photonic device.

Scientific Approach

The Northwestern team has developed a numerical approach that applies optimal control theory as a design tool to produce nanophotonic devices with desired functions. The tool is being used to optimize the coherence properties of laser radiation as well as the structural parameters of the material system to yield desired results.

Researchers are combining two numerical techniques, complemented by analytical methods.

The first is a finite-difference time-domain (FDTD) method to simulate the transport of electromagnetic energy by solving relevant Maxwell equations in the presence of nanoparticle arrays embedded in different media.

The second is a genetic algorithm search technique, a numerical optimization method inspired by the biological process of evolution.

Under the DOE INCITE program, the team used the Blue Gene/L computer at the Argonne Leadership Computing Facility to provide the computational horsepower needed to apply and refine its research approach.

Research Results

Recent research results include design of an optimized nanoscale metallic lens that can focus a field of electromagnetic (EM) radiation into a desired point in space. An important recent result is the design of a periodic array that changes the polarization properties of an incident plane wave in a desired fashion.

Other work has produced accurate near-field simulations, required for the proper design of tip-enhanced Raman-scattering spectroscopy—use of a tiny needle-like tip for improved materials analysis.

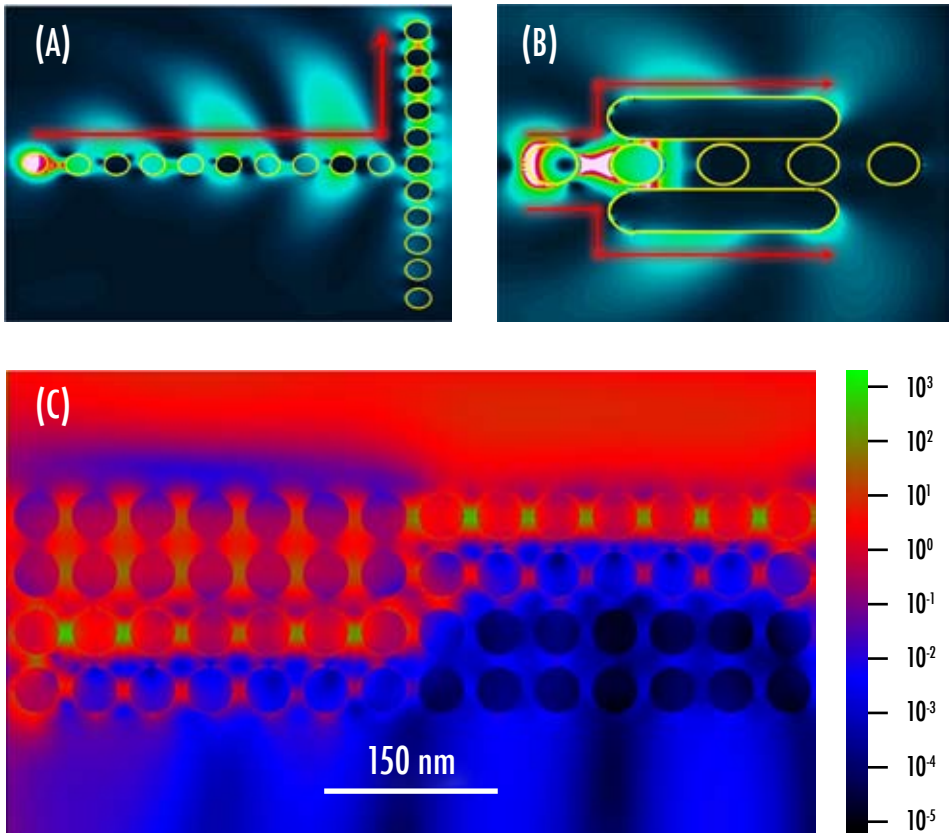
Researchers also have explored L-shaped nanoparticles, associating for the first time an observed high-energy resonance with volume plasmon oscillations due to geometrical asymmetry of the particle.

Looking Ahead

Researchers will study hybrid constructs—such as a combination of nanoparticles and nanowires to achieve both longer-distance (several micrometers) transmission and coherent control of EM energy while minimizing losses. They will develop a nanoplasmonics-based approach for improved solar energy conversion.

Another initiative will aim to develop a general tool to focus and trap quantum objects (atoms and molecules) using nanostructures made of composites previously not studied.

A third research area is the potential for coherent control of light by a mechanism called plasmon-assisted trapping, using crystal structures.



Researchers are applying coherent control tools and concepts to guide and manipulate light in the nanoscale.

The T-junction in Panel A is designed to guide EM energy traveling down the leg into one or the other of the two symmetry-equivalent arms of the junction. The challenge of inducing light to bend about corners is achieved by choice of the incident field polarization. The symmetry breaking is achieved by choice of the incident field phase.

Panel B depicts a hybrid construct, which combines elements that provide local enhancement (such as nanospheres) with elements that provide long-distance propagation (such as nanowires) in order to minimize losses. The structural parameters of the construct are optimized using a genetic algorithm.

Panel C depicts a plasmonic nanocrystal, developed to separate an incident plane wave into two frequency components and funnel each component in a different direction normal to the direction of incidence, in parallel to the surface plane.

"Combining highly parallelized FDTD simulations with optimal control techniques is a numerically challenging research approach. Our partnership with Argonne through the INCITE program has allowed us to explore modeling and analytical methods more rapidly and efficiently than would otherwise have been possible."

Tamar Seideman
Northwestern University

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physical chemistry

What Happens to Water in Confined States?

Researchers:

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University of California—Davis

Jeffrey Grossman
University of California—Berkeley

François Gygi
University of California—Davis

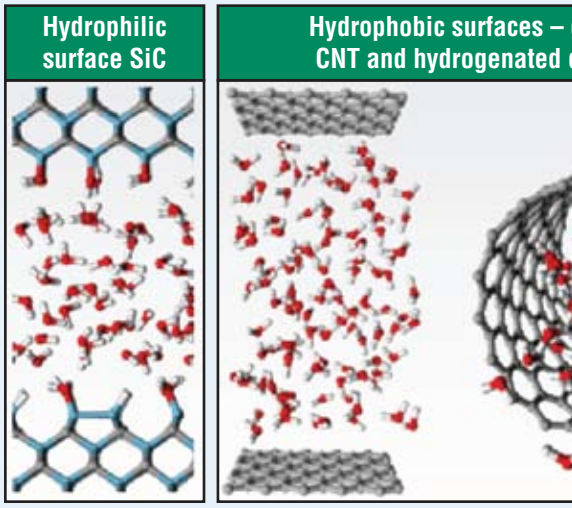
Eric Schwegler
Lawrence Livermore National Laboratory

In the last decade, water in confined environments (see figure) has attracted considerable attention due to its relevance to many systems in diverse fields of science, including biology, nanofluidic devices, inorganic materials, and geology. For example, in cell membranes, key phenomena taking place in aqueous solutions occur in confined geometry: Proteins such as acquaporins are believed to transport water in a very fast way due to the presence of a channel in their secondary structure, where water is confined. In materials science, confined water is found in clays and cements but also in zeolites that are characterized by the presence of cylindrical pores with diameters as small as 7 Å. Zeolites have been widely investigated for their catalytic activity, and changes in the solvation properties of water molecules are expected to influence the thermodynamic equilibrium of solvent-driven reactions. Yet it is poorly understood how chemical reactivity is influenced under confinement.

An important general question on confined water concerns the influence of the confining medium and, in particular, the impact of the hydrophobic (hydrophilic) character of the confining surface on the structural, electronic, and dynamical properties of the liquid. Does a confined phase of water exist that is independent of confining surfaces, or does the presence of an interface represent the dominant influence on the properties of the nanoscale liquid?

Scientific Approach

Experimentally, structural properties of water confined by both hydrophilic and hydrophobic media have been mostly studied by means of X-ray and neutron diffraction techniques, which give access to pair correlation functions. Interpreting experimental results on confined water has proven rather difficult in many instances, and firm conclusions based only on experimental observations are sometimes hard to draw. For this reason, atomistic simulations are often performed in parallel with experiments. Atomistic simulations represent a unique and powerful tool to describe, in a microscopically detailed way, changes in hydrogen bond patterns, molecular preferential orientation, and translational and rotational dynamics. Simulations can be employed to obtain low energy structures, or to calculate, through molecular dynamics, statistical ensemble averages and thermodynamic quantities, and to extract quantities directly comparable to experiments (e.g., pair correlation functions, infrared spectra, bond lifetimes, etc.).



Examples of the various water confinement configurations.

"When attempting to solve challenging problems using computational tools, especially in the presence of controversial and contradicting experimental results, the only way to possibly succeed is to have dedicated time to carry out cutting-edge, thorough studies at a sustained pace. This is exactly what INCITE grants provide us with."

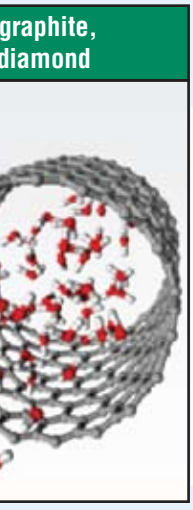
Giulia Galli
University of California—Davis

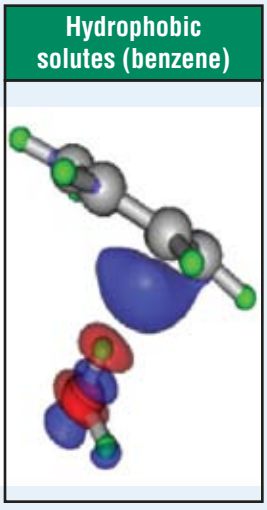
Research Results

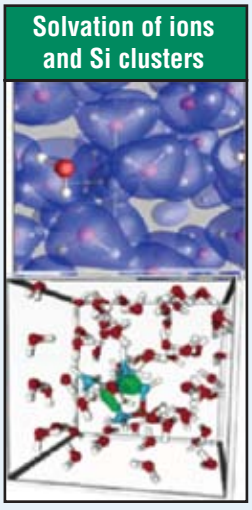
In 2007, the research team determined the effect of the surface electronic structure on the properties of water in confined states of graphene (a single planar sheet of bonded carbon atoms) and carbon nanotubes. These results would not have been possible without an INCITE allocation. The team used the allocation to run calculations on the IBM Blue Gene/L supercomputers at the Argonne Leadership Computing Facility and IBM's T.J. Watson Research Laboratory. Research conclusions stemmed from the results of several different sustained runs carried out over a number of months.

Looking Ahead

The researchers will complete *ab-initio* simulations of ions in confined water, in particular, alkali and halogen ions in water confined in carbon nanotubes. They will also begin calculations of Raman spectra of water, in addition to infrared spectra simulations, as well as calculations of water confined by substrates with electronic properties different from those of graphite and nanotubes. Electric field calculations will use a new version of Qbox optimized to compute localized Wannier functions (i.e., quantities needed to do calculations in electric fields). Tests of the new version of the code are under way.







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life sciences

Scientists Gain Insight into Molecular Basis of Parkinson's Disease

Researchers:

Igor Tsigelny
University of California—San Diego/SDSC

Mark Miller
University of California—San Diego/SDSC

Eliezer Masliah
University of California—San Diego

Through their DOE INCITE project, scientists from the San Diego Supercomputer Center (SDSC) at the University of California–San Diego (UCSD) gained valuable insight into the molecular mechanism of Parkinson's disease progression. The team's work has provided a test bed for identifying possible therapeutic interventions through computational modeling and has broad applicability to other diseases. The test bed offers a computational framework for generating hypotheses about treatments that can be adapted readily to state-of-the-art, high-throughput virtual screening of pharmacophores as potential lead compounds. Academic and pharmaceutical companies could use such a modeling system for further testing and improving potential pharmacophores and other palliative therapies.

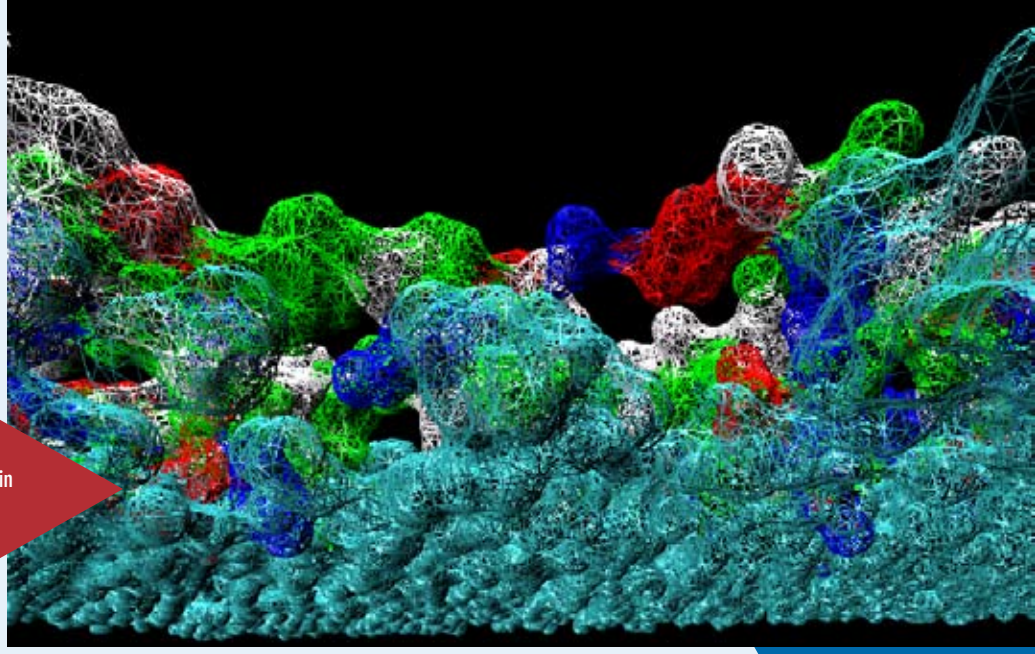
Processor-hour allocations from the INCITE program allowed the SDSC team to perform complex calculations for the research on high-performance Blue Gene/L computers at the Argonne Leadership Computing Facility (ALCF) and SDSC. At the ALCF, researchers used a 2,048-processor, 5.7-teraflops Blue Gene/L dedicated to a mix of INCITE projects and scalable software evaluation and development projects. At the SDSC, they used a 6,144-processor, 13.8-teraflops IBM Blue Gene/L computer.

Scientific Approach

The researchers conducted a comprehensive investigation of aS penetration into the membrane, including a thorough study of pore creation. In this endeavor, larger simulations focused on the interaction of higher-level aS oligomers with the membrane, which increases the number of atoms in the system up to approximately 800,000. The team employed a computational approach that used the NAMD molecular dynamics package, along with the MAPAS program and a set of docking programs on the Blue Gene/L computer system. Together, the programs enabled SDSC researchers to make predictions for conformational changes of proteins, explore protein-protein interactions and/or aggregation, and study interaction of proteins individually or as a complex with the membrane.

"The present study—using molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis—shows that alpha-synuclein can lead to the formation of pore-like structures on membranes. In contrast, beta-synuclein or b-synuclein appears to block the propagation of alpha-synucleins into harmful structures."

Igor Tsigelny
University of California—San Diego/SDSC



A membrane (cyan, cut from the bottom) embedded with the residues of alpha-synuclein pentamer (cut at the top on the level of the highest membrane atom).

Research Results

Using molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis, the team showed that increased aggregation of a protein known as alpha-synuclein (aS) can lead to the formation of harmful pore-like structures in human membranes (see figure). In contrast, beta-synuclein (bS) appeared to block the propagation of alpha-synuclein into the structures.

Given the encouraging correlation between the molecular dynamics modeling predictions and laboratory experimental results, the team expects to make steady progress with the computational model for Parkinson's disease progression and develop cues for design of effective drugs based on computational modeling and simulations.

The computational work conducted in this research also offered significant benefits in driving the creation of new simulation capabilities. It required the researchers to adapt existing tools for molecular simulation to the new Blue Gene architecture. The architecture was unique in providing a very large and dense processor array, using relatively less memory per computational node. As a result, the strategies for running simulations on this platform required the adaptation of existing community codes to a new computing paradigm. For example, the community code CHARMM required the full list of data objects to be resident on each node, a strategy that might not work well on the Blue Gene. Efforts are under way at SDSC, IBM, and elsewhere to adapt codes like this to petascale platforms.

Looking Ahead

The research team will focus on a more comprehensive investigation of alpha-synuclein penetration into the membrane, including a thorough study of pore creation. The scope of the team's work has increased in both the number of simulations being conducted and the scale of the simulations.

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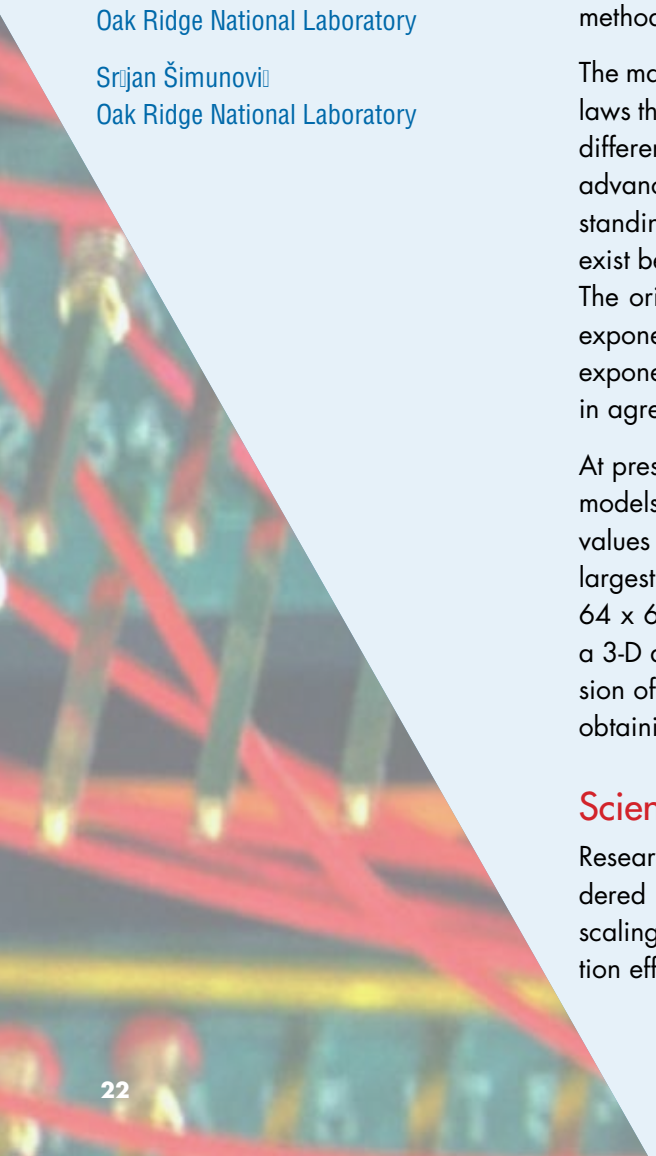
materials science

Blue Gene Simulations Shed Light on Scaling Laws Governing Materials Fracture

Researchers:

Phani Nukala
Oak Ridge National Laboratory

Srđjan Šimunović
Oak Ridge National Laboratory



Understanding how materials fracture is a fundamental challenge of science and engineering. Some key questions about material fracture include 1) what are the size effects and scaling laws of fracture of disordered materials? and 2) how can the fracture surfaces of materials as different as metallic alloys, glass, wood, and mortar be so similar?

Material disorder and long-range interactions are two key components that complicate the study of material failure. From a practical point of view, the main issue associated with the fracture of quasi-brittle materials (such as concrete and ceramics) is the scaling of material strength–how properties like strength scale with sample size, also known as the size-effect. Understanding the size-dependence of material strength and its sample-to-sample statistical fluctuations is crucial to the design and failure analysis of engineering structures involving these materials.

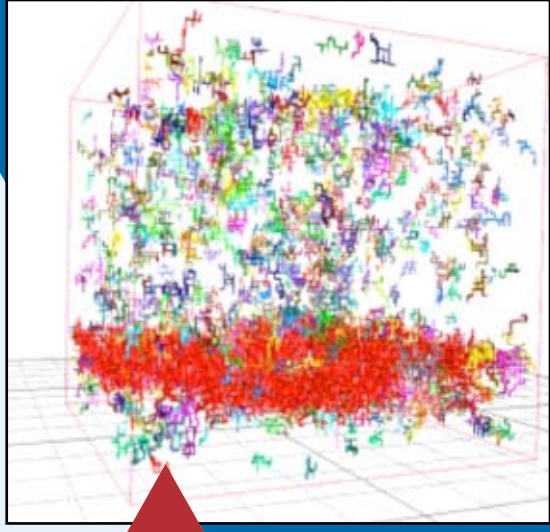
On the other hand, the relation between fracture and phase transitions poses many fundamental questions in statistical physics. Experimental results reveal the existence of an intriguing crackling noise in the acoustic emission and of self-affine fractals in the crack surface morphology. Understanding the acoustic emission signatures associated with the crackling noise of fracture experiments serves as a methodology for forecasting impending structural failure.

The main theoretical challenge, however, lies in understanding the generic scaling laws that govern fracture of materials. It is intriguing that fracture surfaces of many different materials exhibit the same universal roughness characteristics. Recent advances in computer power have enabled considerable progress in the understanding of such models. Despite these advances, many controversial issues still exist between theoretically estimated results and experimentally measured values. The origin of both the scaling and universality of the fracture surface roughness exponent lies at the heart of the controversy. Theoretically estimated roughness exponents of three-dimensional (3-D) fracture surfaces and planar cracks are not in agreement with the experimentally measured values.

At present, simulations on larger system sizes using more complicated theoretical models are necessary to bridge this gap between the experimentally observed values and the theoretical estimates. Despite recent algorithmic advances, the largest 3-D lattice system fracture simulation has been limited to system sizes up to 64 x 64 x 64, since the CPU time required to analyze the fracture simulation of a 3-D disordered lattice system increases as O(L6.5), where L is the linear dimension of the 3-D lattice system. Simulations of much larger systems are required for obtaining accurate scaling laws in 3-D.

Scientific Approach

Researchers at Oak Ridge National Laboratory pursued the largest ever 3-D disordered lattice systems (size 1283) through their DOE INCITE award to obtain the scaling laws of fracture surfaces. This effort required over 90 times the computation effort of size 643.



Simulated crack cluster and fracture surface.

The team developed an algorithm based on a block-circulant preconditioned conjugate gradient (CG) iterative scheme for simulating 3-D random fuse and beam networks. The new algorithm significantly reduced the computational time required for solving large lattice systems in comparison with the Fourier accelerated iterative schemes used for modeling lattice breakdown. With the block-circulant preconditioner, the researchers were able to simulate fracture in lattice systems of sizes up to 128 x 128 x 128 on a 1,024 IBM 1.3 GHz Power4 processor. The simulation began with an intact lattice system and was carried out by breaking one bond at a time until the macroscopic fracture occurred. Simulations were conducted on the IBM Blue Gene/L computer at the Argonne Leadership Computing Facility.

Research Results

Using large-scale numerical simulations on the BG/L, researchers accomplished the following during FY07:

- Achieved large-scale simulation of beam lattice systems to understand the universality, anomalous, and multi-affine scaling features of fracture surface roughness.
- Developed a novel scaling law for material strength that captures, for the first time, the experimentally observed crossover from a stress concentration-controlled scaling regime to a disorder-controlled scaling regime. The scaling law is in excellent agreement with the experimental data on notched paper samples. This universal scaling law extended researchers' understanding of size dependence of material strength and is relevant for the design and analysis of engineering structures made up of quasi-brittle materials.
- Multi-affine scaling of fracture surfaces is an artifact of jumps in the crack profiles. Numerical results indicated that apparent multiscaling of crack surface roughness observed at small scales is due to the removal of overhangs of the fracture surfaces and that the roughness crosses over to self-affine scaling at large scales.
- Anomalous scaling is a generic feature of fracture simulations obtained using fuse models. Removing the jumps in the crack profiles does eliminate this anomalous scaling. However, simulations using beam lattice systems indicate that crack roughness does not exhibit anomalous scaling in sharp contrast to the simulation results obtained using scalar fuse lattices.
- Researchers' largest-ever system size simulations with extensive statistical sampling indicated that the local roughness exponent is independent of disorder strength and initial notch size.

Looking Ahead

Researchers intend to investigate the fracture of notched 3-D beam lattice systems to understand anisotropy of fracture roughness exponents and size effect on material strength.

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gearing up for Blue Gene/P

The Argonne Leadership Computing Facility (ALCF) made tremendous progress during 2007 in meeting key objectives and establishing core capabilities to fulfill its longer-term mission. Major milestones were achieved on several fronts, including scientific impact, facility build-out, organizational expansion, improving operations, and outreach.

Much of FY07 was spent establishing a solid foundation for the facility at Argonne National Laboratory. FY08 represented a year of continued expansion in organizational and system capabilities. With this expansion, the ALCF became a critical national resource for meeting the growing demand of large-scale computing in support of breakthrough science and engineering research.

The ALCF and Argonne National Laboratory coordinated efforts for the build-out of the Interim Supercomputing Support Facility (ISSF), which achieved beneficial occupancy in July. The ALCF team worked closely with IBM on installing the 111-teraflops Blue Gene/P system in late 2007 and the 445-teraflops Blue Gene/P system in mid-2008 in the ISSF.

Organizational Developments

The ALCF team grew considerably in 2007. The core management team was established. Key hires took place in operations, applications performance engineering and computational science, user services and outreach, and administration. The culture of "customer advocacy" and "continuous innovation" was further strengthened. The ALCF team was well positioned to work closely with INCITE project teams and provide expert assistance and support in maximizing the impact of supercomputing capabilities on many areas of scientific and engineering discovery.

DOE INCITE Program Support

The number of DOE INCITE projects awarded to the ALCF continues to increase each year. In 2006, the ALCF supported six INCITE projects. In 2007, the number of supported INCITE projects grew to nine, spanning computational biosciences, combustion modeling, climate modeling, nanoscale science, materials science, nuclear engineering, and life sciences. In 2008, 20 INCITE projects were awarded more than 111 million hours of computing time on the Blue Gene/P at the ALCF in a diverse range of scientific disciplines (see pages 28-29).

ALCF collaboration with INCITE projects has been marked by high levels of end-user satisfaction and significant scientific progress made by the research teams.

Collaboration has taken the form of:

- Application performance engineering assistance to researchers;
- Providing training on system usage, system architecture, etc., through one-on-one sessions and workshops;
- Jointly developing articles with researchers to highlight scientific achievements and progress;
- Problem-solving with users and developers of scientific applications;
- Creating awareness of the DOE INCITE program and providing assistance to pioneer science projects.

Installed in 2007-08 at the ISSF, the IBM Blue Gene/P supercomputer was designed to meet both compute and data needs at the petascale level.

Facilities and Operations

In FY07, ALCF successfully completed project baselining and planning reviews. The overall project effort continued to proceed according to schedule and within budget. ALCF and Argonne National Laboratory coordinated their efforts for the build-out of the Interim Supercomputing Support Facility (ISSF), which achieved beneficial occupancy in July. The ALCF team worked closely with IBM on installing the 111-teraflops Blue Gene/P system in late 2007 and the 445-teraflops Blue Gene/P system in mid-2008. The system architecture was designed to meet both compute and data needs at the petascale level. ALCF operations started to move from the "establishment" phase to the "maturity" and "continuous improvement" phases. In preparation, key processes have been formalized and streamlined, and staff are developing and deploying complementary system support and system management tools.

Planning for Growth

Requests for INCITE allocations on the Blue Gene in 2007 greatly exceeded available resources—a trend expected to continue. Goals for FY08 focused on expanding the ALCF's capabilities to support breakthrough science and engineering on a larger scale. Demand from the scientific research community for petascale systems in general, and IBM Blue Gene capacity in particular, was very high and continued to grow. With the significant expansion of ALCF Blue Gene system resources under way, a larger number of leading research efforts can be supported, fulfilling ALCF's vision as a world-class center for computation-driven scientific discovery.

outreach

ALCF Activities Draw INCITE Users, Colleagues, and Students

In 2007, Argonne Leadership Computing Facility (ALCF) staff educated and informed INCITE researchers, supercomputing colleagues, and students through a variety of outreach activities, including workshops, conference exhibits and posters, and a job fair.

Blue Gene INCITE Workshop Offers Jump Start on Resource Use

The ALCF Blue Gene INCITE Workshop held February 7-8 at Argonne helped new INCITE project awardees get a quick start on the use of resources and services offered by the ALCF. The workshop offered both a presentation and hands-on format to maximize interactions between INCITE project teams and ALCF staff.

Participants successfully compiled and executed their research code at the workshop. Several optimizations also were attempted, and some scale-out simulations were performed. Together, the ALCF teams and research teams established a good understanding of areas needing further investigation and collaboration to help maximize performance on the IBM Blue Gene/L in support of their research.

Poster Features ALCF Research at CSGF Program Annual Meeting

ALCF research was featured in a poster displayed at the 2007 Department of Energy Computational Science Graduate Fellowship (CSGF) Conference on June 19-21 in Washington, D.C. The annual gathering, which drew 175 attendees in 2007, is the largest opportunity for fellows to meet each other and present their research to government officials, members of national laboratory communities, alumni, and each other. The conference featured talks by fellows, a fellows poster session, and a poster display showcasing the national labs.

June Workshop Gives Guidance on INCITE Proposal Writing

On June 20-21, 35 participants from national labs, industry, and academia attended the INCITE Next-Generation Blue Gene Workshop hosted by the ALCF and the BlueGene Consortium at Argonne. The workshop provided current and prospective DOE INCITE project teams with an understanding of DOE's INCITE program, suggestions on how to write a successful INCITE proposal, and visibility into the review process. It also covered the ALCF and its relationship with the INCITE program. Given Argonne's use of the IBM Blue Gene system at the ALCF, discussions focused on the system and its capabilities.

ACM Job Fair Informs Students about ALCF Opportunities

ALCF staff discussed computing science opportunities and internships with students who attended a job fair held at the 13th Annual Reflections | Projections Computing Conference hosted by the Association for Computing Machinery at the University of Illinois. Approximately 500 students tapped into the Oct. 12th fair, located at the University of Illinois at Urbana-Champaign campus in the new Thomas M. Siebel Center for Computer Science.

The job fair featured 25 premier computing and technology employers offering internships and full-time employment. Employers included Amazon.com, Argonne National Laboratory, Bank of America, Beckman Coulter, E*Trade Financial, EA, Facebook, General Electric, Goldman Sachs, Google, Intel, International Game Technology, Lime Wire, Lockheed Martin, Microsoft, Morgan Stanley, Navteq, NVIDIA, Palantir Technologies, Riverbed Technology, Roundarch, Salesforce.com, VMware, Volition, and Yahoo.

ALCF Hosts Exhibit at Grace Hopper Celebration of Women in Computing

The ALCF hosted an exhibit at the seventh Grace Hopper Celebration of Women in Computing Conference on October 17-20 in Orlando, Fla. The conference is designed to bring the research and career interests of women in computing to the forefront. Conference presenters are leaders in their respective fields, representing industry, academia, and government. Top researchers present their work, while special sessions focus on the role of women in today's technology fields. The 2007 conference sold out, with 1,430 in attendance. Women from more than 23 countries, 212 universities, and 93 companies participated in the event.

SC07 Spotlights INCITE Research Conducted on Blue Gene/L

At SC07 on November 10-16, ALCF presentations focused on Argonne, Procter & Gamble, and Pratt & Whitney INCITE projects under way on the Blue Gene/L. In addition, presentations were given on other cutting-edge developments in high performance computing. A set of electronic posters displayed dynamic views of the research being conducted at the ALCF.

2008 INCITE projects

In 2008, the DOE INCITE program awarded 20 research projects more than 111 million hours of computing time on the next-generation IBM Blue Gene/P system at the Argonne Leadership Computing Facility.

Applied Mathematics

Reactor Core Hydrodynamics

Paul Fischer, Argonne National Laboratory
Blue Gene Hours: 14,000,000

Astrophysics

Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models

Don Lamb, ASC/Alliance Flash Center, University of Chicago
Blue Gene Hours: 21,000,000

Chemical Sciences

Molecular Simulation of Complex Chemical Systems

Christopher Mundy, Pacific Northwest National Laboratory
Blue Gene Hours: 750,000

Chemical Sciences

Molecular Simulations of Surfactant-Assisted Aqueous Foam Formations

Kelly Anderson, Procter and Gamble
Blue Gene Hours: 4,000,000

Climate Research

Climate-Science Computational End Station Development and Grand Challenge Team

Warren Washington, National Center for Atmospheric Research
Blue Gene Hours: 1,000,000

Combustion

Massively Parallel Simulation of Combustion in Gas Turbines

Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Blue Gene Hours: 4,000,000

Computational Proteomics

Computational Protein Structure Prediction and Protein Design

David Baker, University of Washington
Blue Gene Hours: 12,000,000

Computer Sciences

Blue Gene/P Plan 9 Measurements on Large-Scale Systems

Ronald Minnich, Sandia National Laboratories
Blue Gene Hours: 1,000,000

Computer Sciences

Performance Evaluation and Analysis Consortium End Station

Patrick Worley, Oak Ridge National Laboratory
Blue Gene Hours: 4,000,000

Engineering Physics

High-Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability

Peter Bradley, Pratt and Whitney
Blue Gene Hours: 1,377,000

Fusion Energy (Plasma Physics)

High-Resolution Global Simulation of Plasma Microturbulence

William Tang, Princeton Plasma Physics Laboratory
Blue Gene Hours: 2,000,000

Lattice Gauge Theory

Lattice QCD

Robert Sugar, University of California, Santa Barbara
Blue Gene Hours: 19,600,000

Life Sciences

Gating Mechanism of Membrane Proteins

Benoit Roux, Argonne National Laboratory and The University of Chicago
Blue Gene Hours: 1,500,000

Life Sciences

Large-Scale Simulations of Cardiac Electrical Activity

Jeffrey Fox, Gene Network Sciences
Blue Gene Hours: 846,720

Life Sciences

Simulation and Modeling of Synuclein-based "Protofibril Structures" as a Means of Understanding the Molecular Basis of Parkinson's Disease

Igor Tsigelny,
University of California-San Diego
Blue Gene Hours: 1,200,000

Materials Science

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles

Christopher Wolverton, Northwestern University
Blue Gene Hours: 1,000,000

Materials Science

Modeling the Rheological Properties of Concrete

William George,
National Institute of Standards and Technology
Blue Gene Hours: 750,000

Nuclear Energy

Predictions of Thermal Striping in Sodium-Cooled Reactors

Andrew Siegel, Argonne National Laboratory
Blue Gene Hours: 5,000,000

Nuclear Physics

Computational Nuclear Structure

David Dean, Oak Ridge National Laboratory
Blue Gene Hours: 10,000,000

Physical Chemistry

Water in Confined States

Giulia Galli, University of California
Blue Gene Hours: 6,000,000

2008 ALCF facts & figures

What is the mission of the ALCF?

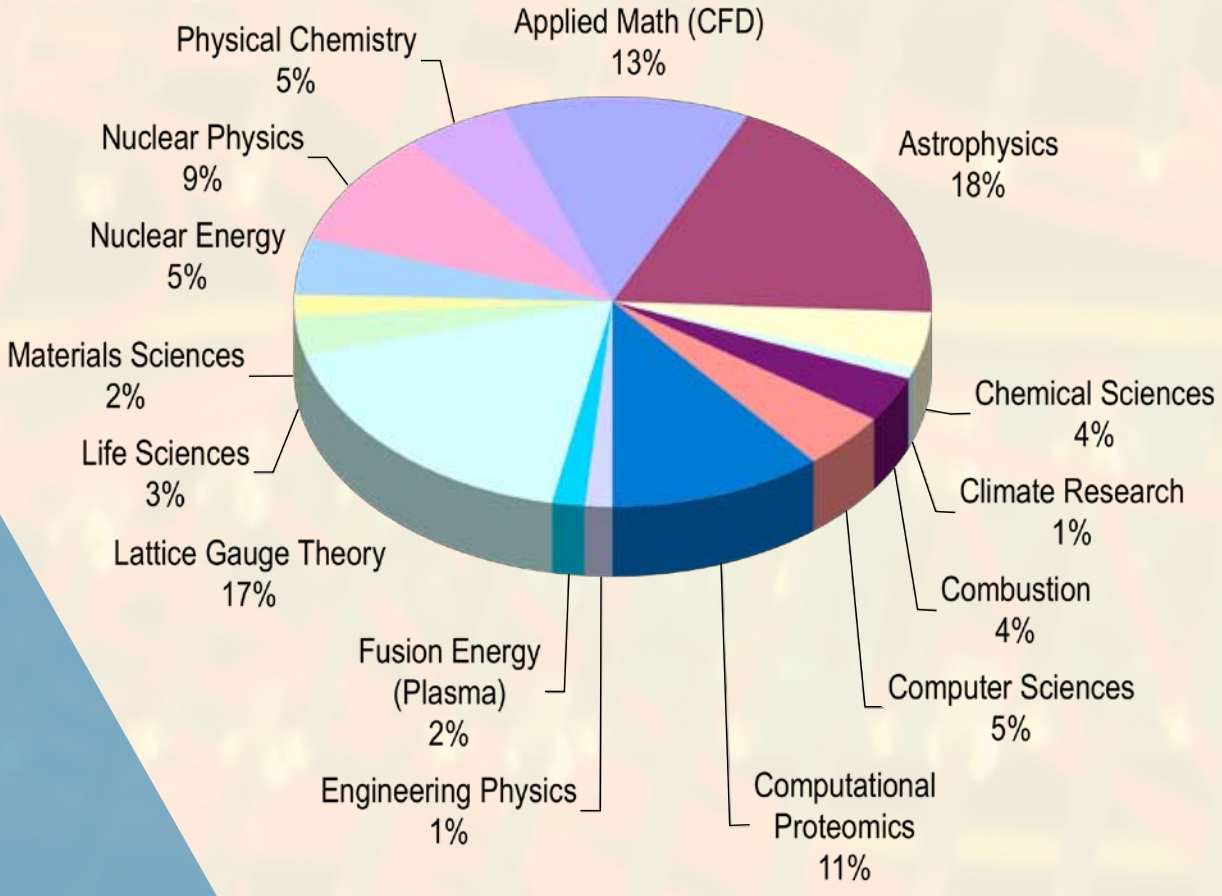
Established in 2006, the Argonne Leadership Computing Facility (ALCF), located at Argonne National Laboratory, provides the computational science community with a leading computing capability dedicated to breakthrough science and engineering.

What research is being conducted at the ALCF?

In 2008, researchers are using the IBM Blue Gene/P at the ALCF to conduct 20 projects with a total of 111 million hours of computing time. The research encompasses a diverse span of scientific domains (see pie chart). It ranges from large-scale simulations of potentially dangerous heart rhythm disorders to running detailed numerical experiments of thermal striping in sodium-cooled fast reactors.

How are research projects selected?

The U.S. Department of Energy's Office of Science selects major ALCF projects through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This program seeks computationally intensive research projects of the largest scale that can make high-impact scientific advances through the use of a major allocation of computer time, resources, and data storage.



What resources does the ALCF offer to users?

The ALCF provides the following IBM Blue Gene systems:

Intrepid, an IBM Blue Gene/P system, is used primarily for production scientific and engineering computing. It achieves a peak speed of 557 teraflops and a Linpack speed of 450 teraflops. Intrepid's configuration features 40,960 nodes, each with four processors or cores for a total of 163,840 cores and 80 terabytes of memory.

Most applications that run on large-scale systems like Intrepid generate huge volumes of data that represent the results of the calculations. Intrepid's data systems consist of 640 I/O nodes that connect to 16 storage area networks (SANS) that control 7,680 disk drives with a total capacity of over 6 petabytes and an aggregate transfer speed of 80 gigabytes per second.

An essential tool for understanding the results after the run has completed is the ability to rapidly explore the output data and convert it to a visual representation. To do so at the scale required by Intrepid's applications requires a system with significant power. A new supercomputer installation, nicknamed Eureka, will allow researchers to explore and visualize the data they produce with Intrepid. The NVIDIA Quadro Plex (S4) visual computing system is the base graphics building block for the installation and the largest installation of its kind in the world. Eureka offers 104 dual quad core servers with 208 Quadro FX5600 graphics processing units (GPUs) in the S4s.

Two parallel file systems—PVFS and GPFS—manage data storage. An HPSS automated tape storage system provides archival storage.

The ALCF also operates Surveyor, a Blue Gene/P system with 1,024 quad-core nodes (4,096 processors) and 2 terabytes of memory. Surveyor is used primarily for tool and application porting, software testing and optimization, and systems software development. Peak performance is 13.9 teraflops.

What user support is available?

The ALCF provides a help desk to assist users with their applications. ALCF Service Desk staff is available from 9 a.m. to 5 p.m. (Central Time) Monday through Friday for support. In addition, the Service Desk offers emergency support via e-mail after regular hours and during weekends. Hands-on workshops also are provided to assist users with their applications.

How can I submit a project?

Each year, scientists, universities, and industry can submit a project for consideration through the peer-reviewed INCITE program. For more information about the INCITE program and proposal submittal, refer to the DOE website.

Whom can I contact at the ALCF for more information?

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ALCF Acting Division Director
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The Argonne Leadership Computing Facility was dedicated on April 21, 2008 during a ceremony attended by key federal, state, and local officials.

UChicago ▶ Argonne LLC

Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

alcf-annrep-1108

accelerating scientific discovery