2008 INCITE Highlights

Predicting Structures of Biologically Important Proteins
Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires a detailed picture of their structure. To address this challenge, a research group led by David Baker at the University of Washington has developed and is using the ROSETTA method for computationally predicting protein structure. The group's goal is to create detailed, three-dimensional models of the structure of selected proteins at atomic-level resolution. Under the INCITE program, the team is refining and expanding the capabilities of the ROSETTA method by using the Blue Gene/P at the Argonne Leadership Computing Facility. Over the past year, the method has been tested on several proteins of known structure up to 189 amino acids in length. In many cases, the accuracy of the prediction was within a remarkable one angstrom of the experimentally solved high-resolution crystal structure. Currently, the method is being tested on proteins of known structure to determine the size range and fold classes for which accurate results can be predicted. Subsequent computations will focus on making predictions for proteins with unknown structures. Additional work will go into refining the method to expand the range of proteins to which it can be applied.

INCITE Allocation: 12 million processor hours (Blue Gene/P at ANL)

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

—David Baker, University of Washington

Interaction of Turbulence and Chemistry in a Low Swirl Burner
New combustion systems based on ultra-lean premixed combustion have the potential for dramatically reducing pollutant emissions in transportation systems, heat and stationary power generation. However, lean pre-mixed flames are highly susceptible to fluid-dynamical combustion instabilities, making robust and reliable systems difficult to design. Low swirl burners are emerging as an important technology for meeting design requirements in terms of both reliability and emissions for next generation combustion devices.

Using their INCITE award, a team from Lawrence Berkeley National Laboratory led by John Bell has performed simulations of a laboratory-scale low swirl burner using detailed chemistry and transport without incorporating explicit models for turbulence or turbulence/chemistry interaction We modeled two different fuels, methane and hydrogen, each at two turbulent intensities. The simulations were done using a parallel adaptive low Mach number combustion code LMC with an INCITE grant for computational resources at NERSC. The combination of adaptive mesh refinement, a low Mach number formulation and the computational resources available through INCITE enabled us to perform simulation in a 25 cm^3 domain with an effective resolution of 2048^3.

INCITE Allocation: 3,384,615 processor hours (NERSC HPC at LBNL)

"INCITE has been essential to our research on hydrogen combustion. Without the computational resources provided by INCITE we would be unable to simulate flames at the realistic laboratory conditions needed to understand their behavior,"

—John Bell, Lawrence Berkeley National Laboratory

Improving Aircraft Engine Combustor Simulations

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. Pratt & Whitney (P&W) has been exploring leading-edge combustor design methods using the Blue Gene/P supercomputer at the Argonne Leadership Computing Facility. 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. The research has led to improved capabilities and reduced solution times for 3-D combustor simulations. It has been a key enabler for the depth of understanding needed to meet emissions goals. Capabilities improved through the INCITE allocations are now being applied to P&W's next-generation, low-emission PurePower™ engine.

INCITE Allocation: 1,377,000 processor hours (IBM Blue Gene/P at ANL)

"Pratt & Whitney is developing a groundbreaking new engine known as PurePower™. This engine will deliver double-digit reductions in fuel consumption, emissions, and cost of ownership. Advances made under the INCITE program are now contributing to this industry-changing product."

—Peter Bradley, Pratt & Whitney

Gyrokinetic Steady State Transport Simulations

The fundamental scientific advance targeted in this project is the multi-scale simulation of a burning plasma core for the International Thermonuclear Experimental Reactor (ITER) in particular. Plasma creates energy when hydrogen atoms collide, resulting in high-energy alpha particles that heat the plasma but can be ejected by turbulence of the gas. Turbulence is necessary for a tokamak reactor. The GYRO code employed in these simulations computes "optimal turbulence," finding the perfect balance of heat and alpha-particle production and loss. This multi-scale simulation will be used to predict the performance given the temperature and density, which is critical to the design of diagnostics and the selection of operating points for the ITER project, a prototype fusion reactor that could lead the way to commercially viable fusion power. Fusion power, if mastered, could one day provide the world with a virtually unlimited energy source free of harmful emissions and with reduced nuclear storage and proliferation risks.

INCITE Allocation: 1,500,000 processor hours (Cray XT4. OLCF)

"The key is to know the rate at which the plasma is leaking heat and particles, because while some loss is necessary, too much can be detrimental."

–Jeff Candy, General Atomics

Simulating Binary Black Holes and Gravitational Radiation

The final stage of massive black hole (MBH) binary evolution is a strong source of gravitational waves for laser-interferometric observatories. A full theoretical understanding of the merger, as predicted by General Relativity, is essential for realizing the scientific potential of these observations. Dramatic advances have recently been made in numerical relativity techniques for binary black hole simulations with adaptive mesh refinement (AMR), greatly expanding the scope of problems which can be profitably investigated. NCCS resources were used in this project led by Joan Centrella of NASA's Goddard Space Flight Center to apply these techniques to model the astrophysical coalescence of comparable mass MBH binaries for different mass ratios and spins, and calculate the resulting gravitational wave signatures. The objectives of the experiment were to understand the dynamics of (comparable mass) binary black hole mergers for astrophysically interesting mass ratios and spins; to compute and characterize the resulting gravitational waveforms; and to investigate astrophysical applications.

INCITE Allocation: 1,000,000 processor hours (Cray XT4. OLCF)

The Role of Eddies in the Meridional Overturning Circulation

This project contributed to understanding fundamental dynamics of ocean circulation driven by differences in the temperature and salinity of sea water. Using high-resolution models of the ocean component of the Earth's climate system, the researcher team led by Paola Cessi of the University of California, San Diego examined processes that maintain the abyssal circulation of the ocean to understand its response to changes in atmospheric composition. Meridional overturning circulation—sometimes called the ocean conveyer belt—is an essential component of the ocean-atmosphere heat budget and a major player in sequestering carbon dioxide into the deep ocean. It mixes the world's oceans and transports energy and matter around the globe.

Simulations to date have revealed that in the Antarctic Circumpolar Current (ACC), stratication is obtained as a cancellation of the buoyancy transport by the mean, wind-driven circulation and the buoyancy transport by mesoscale eddies. Diapycnal mixing, due to small-scale structures such as breaking internal gravity waves is unimportant for stratification, but directly controls the net buoyancy and heat transports. By systematically varying a series of parameters (the diapycnal diffusivity, the bottom drag, and the surface winds) in the ACC configuration, researchers have been able to establish the dependence of the eddy heat flux on the large-scale buoyancy distribution. With this knowledge, a parameterization of the eddy heat flux has been developed which is consistent with the energy balance and accurately reproduces the direct eddy simulations when used on a coarse grid.

INCITE Allocation: 486,000 hours (Cray X1E, OLCF)

Understanding the Flow of Particles at the Atomic Level
Led by Athonu Chatterjee of Corning, Inc., this project is part of a study to understand the flow of organic molecules and oxide particles in confined geometries at the atomic level. This will help elucidate just how each type of organic additive interacts with each particle type and its impact on the flow of these suspensions. Thus far, their computer simulations using the Hewlett Packard cluster at Pacific Northwest National Laboratory's Environmental Molecular Sciences Laboratory have shown that particle shape affects both how it moves in the suspension and the effect particle charge has.

INCITE Allocation: 750,000 processor hours (HP-MPP at PNNL)

"We are pleased overall with the resources available through the INCITE grant and the services provided. Timely e-mail updates and reminders were very helpful."
Athonu Chatterjee, Corning Inc.

High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels
Supercomputers at the National Center for Computational Sciences (NCCS) are hastening the arrival of advanced combustion devices that will consume less energy and emit fewer pollutants. Mechanical engineer Jacqueline Chen of Sandia National Laboratories (SNL) is leading an effort to simulate the combustion of diverse fuels. The result is a library of science data that captures complex aero-thermo-chemical interactions and provides insight into how flames stabilize, extinguish, and reignite. Chen's data libraries will assist engineers in the development of models that will be used to design next-generation combustion devices burning alternative fuels. With mechanical engineer Chun Sang Yoo of SNL and computational scientist Ramanan Sankaran of ORNL, Chen recently used Jaguar at the NCCS to simulate combustion of ethylene, a hydrocarbon fuel. Their simulation generated more than 120 terabytes (120 trillion bytes) of data—more than ten times as much as contained in the printed contents of the Library of Congress.
The simulation ran a software application developed at Sandia called S3D, which runs on multiple processing cores to model compressible, reacting flows with detailed chemistry. S3D was one of six applications recently selected to run pioneering "science-at-scale" simulations efficiently employing most or all processing cores of Jaguar.

INCITE Allocation: 18,000,000 processor hours (Cray XT4. OLCF)

"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."
–Jacqueline Chen, Sandia National Laboratories

Looking Back at Historical Data to more Accurately Model Future Climate Change
An important consequence of climate change is the altered likelihood of weather extremes. To have confidence in the projected changes of such extremes in the 21st century, it is first necessary to assess model simulations of such changes throughout the 20^{th} century, using daily data. Any such daily verification data must also have quantified estimates of uncertainty to allow a fair quantitative assessment of the simulations. To this

end, through the INCITE program, a team led by Gilbert Compo of the University of Colorado and the National Oceanographic and Atmospheric Administration has embarked upon the Twentieth Century Reanalysis Project. The project is an effort to produce weather maps from the surface of the earth up to the jet-stream level spanning the entire 20th century. The maps are produced using surface observations of subdaily pressure, monthly sea surface temperature and sea ice distribution. These observations are combined using a recently developed Ensemble Filter data assimilation method which directly yields each 6-hourly map as the most likely state of the atmosphere, and also the uncertainty in that map. With the INCITE award, our dataset will provide the first estimates of global tropospheric and stratospheric variability spanning more than 100 years at 6-hourly resolution. This dataset will be used to study climatic variations and trends that could not previously be addressed observationally, such as the 1930's U.S. Dust Bowl, 1920s to 1940s Arctic warming, and trends in severe storms such as the 1922 Knickerbocker snowstorm. Using additional computing power available through INCITE, we have demonstrated that a high-resolution dataset to study historical hurricanes, such as the 1938 Long Island Express Hurricane, can also be produced.

INCITE Allocation: 2,861,538 hours (NERSC HPC at LBNL)

"Without this allocation, we could not be using a state-of-the-art climate model to generate a dataset of the 6-hourly global weather maps spanning 1891 to 2008 that will be used to understand the Dust Bowl and dramatic Arctic warming of 1920-1940s, among other climate and weather extremes of the period."

—Gilbert Compo, University of Colorado

Exploring Nuclear Structure

Researchers are using complementary techniques, including Green's Function Monte Carlo, Hamiltonian Diagonalization (the No Core Shell Model), and Coupled-Cluster methods to perform ab initio calculations of both structural and reaction properties of light and medium mass nuclei and of the three-nucleon force. They are conducting the calculations on the Cray XT4 at Oak Ridge National Laboratory and the IBM Blue Gene/P at Argonne National Laboratory. Their work could provide an ab initio understanding of triple-alpha burning that is essential to life on earth. The project is exploring, for the first time, the role of the three-nucleon force in substantially heavier nuclei such as 160, 40Ca, and 56Ni. The research team is being led by David Dean, Oak Ridge National Laboratory (ORNL), in collaboration with researchers from Iowa State University, University of Tennessee, and Argonne National Laboratory (ANL).

INCITE Allocations: 17.5 million processor hours (Cray XT4 at ORNL: 7.5 million; Blue Gene/P at ANL: 10 million)

"We are performing structure and nuclear reaction calculations for the entire nuclear mass table to improve our understanding of the nuclear energy density functional and to calculate nuclear properties relevant for the description of nuclear reactions, in particular, neutron-nucleus reaction cross-sections and fission. Such calculations are relevant to many applications in nuclear energy and nuclear astrophysics."

—David Dean, Oak Ridge National Laboratory

Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence
Plasma, a ubiquitous form of matter in the universe, is nearly always magnetized and turbulent. If we can understand turbulence in the solar wind streaming past the Earth, then we can understand similar turbulence in the distant universe, such as is found between stars and swirling around supermassive black holes. To understand key data from NASA's Chandra X-ray observatory, one must characterize small-scale, kinetic plasma turbulence. This project leb by William Dorland of the University of Maryland will investigate the properties of magnetized plasma turbulence, a key problem in space physics and astrophysics. It aims to simulate kinetic, low-frequency turbulence in astrophysical plasmas and compare theory and simulation with observation. The goal is to ultimately settle the 40 year old question of the physics beneath the magnetic energy spectrum in the turbulent solar wind through direct numerical simulation of the turbulence at the scale of the ion Larmor radius and to determine the heating of each plasma species resulting from a cascade of balanced Alfven wave turbulence.

INCITE Allocation: 4,000,000 processor hours (Cray XT4. OLCF)

Landmark Direct Numerical Simulations of Separation and Transition for Aerospace
Led by Hermann Fasel of the University of Arizona, this project is conducting landmark direct numerical simulations of two flow problems that are important to the development of new jet engines. The first examines ways in which pulsed vortex generator jets can be used to reattach flows that have become separated from the upper surface of a low-pressure turbine blade; a greater understanding of the process is necessary to move this technology from the laboratory to production jet engines. In the second problem, the team is working to explain the dynamics of coherent structures in Coanda flows, which is crucial for the development of effective and efficient Coanda flow devices.

INCITE Allocation: 400,000 hours (Cray X1E, OLCF)

Making Safe, Clean Nuclear Energy Available Globally
The United States is committed to new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global energy demand. Liquid-metal-cooled fast reactors are a key component of this strategy in that they permit recycling of nuclear fuel and are expected to be economical sources of power. A research team led by Paul Fischer of Argonne National Laboratory, comprised of researchers from Argonne and the University of Illinois, is carrying out large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores. The researchers have simulated wire-wrapped fuel rods with 7-, 19-, and 37-pin bundles on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF). The current computations are some of the largest to date with the spectral element code, Nek5000, and involve several hundred million gridpoints on unstructured meshes. Experiments indicate that low pin count results do not extrapolate to higher pin counts because of the edge channel effects. Succeeding simulations will involve more fuel pins, culminating in the design target of

217 pins. The simulations will enable researchers to gain an understanding of the fundamental thermal mixing phenomena within advanced recycling reactor cores, which can lead to improved safety and economy of these pivotal designs.

INCITE Allocation: 14 million processor hours (IBM Blue Gene/P at ANL)

"Computations on the ALCF Blue Gene/P, made possible through a 2008 DOE INCITE award, are already yielding important results in the analysis and understanding of reactor core flows, including establishment of turbulent flow entry lengths and subassembly coolant mixing characteristics."

—Paul Fischer, Argonne National Laboratory

Preventing Cardiac Rhythm Disorders

In work funded by the National Institutes of Health, a research team led by Jeffrey Fox is using the Blue Gene/P at the Argonne Leadership Computing Facility to rapidly test hypotheses for the initiation and maintenance of cardiac rhythm disorders. The team's large-scale computer simulations represent a promising tool to help identify the underlying electrical mechanisms for dangerous arrhythmias and determine the effects of interventions, such as drugs, that may prevent or exacerbate these arrhythmias. Certain activation sequences have been shown to be particularly effective at inducing arrhythmias in canine experimental models. The research team showed that similar sequences induce wave break, reentry, and sustained fibrillatory activity in a 3-D model of electrical wave propagation in the canine heart.

INCITE Allocation: 846,720 processor hours (IBM Blue Gene/P at ANL)

"Our INCITE award has made the results achieved to date possible. With access to leadership class computational resources, simulations of wave propagation on realistic spatial domains containing tens of millions of spatial grid points can be completed in just a few hours."

—Jeff Fox, Gene Network Sciences

Probing the Properties of Water

Unraveling the properties of water at organic and inorganic interfaces is a key step towards understanding the function of biological systems and the behavior of soft and hard materials in many natural environments. Probing such properties is a very challenging task, both from an experimental and theoretical standpoint. The challenge is even greater if water is confined in very small spaces—within a few nanometers. Exploiting the power of IBM Blue Gene supercomputers at the Argonne Leadership Computing Facility and IBM Blue Gene Watson Research Laboratory, a team of researchers is using first-principles simulations to investigate what happens at the microscopic level when water meets hydrophilic and hydrophobic surfaces and how the properties of this ubiquitous liquid are modified at the nanoscale. The first-principles theory used—density functional theory—yields results that compare well with experiments for all the major structural properties of water, some of its electronic spectroscopic signatures, and several dynamical properties. In addition, the team

identified the key role played by electrons in determining the arrangements of water molecules at the surface. They also computed vibrational spectra and provided predictions and interpretations of what should be seen experimentally when measuring how water molecules vibrate in contact with surfaces. The findings can be applied to solve complex problems in both biology and materials science.

INCITE Allocation: 6 million processor hours (Blue Gene/P at ANL)

"Access to both high performance computing and dedicated queues—and thus, to sustained runs—has been made possible by a DOE INCITE award. For these projects, sustained runs over several weeks were absolutely essential to obtain the results now published in premier journals, including the Proceedings of the National Academy of Science, Physical Review Letters, and Nano Letters."

—Giulia Galli, University of California—Davis

Modeling the Rheological Properties of Concrete

Understanding the mechanisms for the dispersion or agglomeration of suspensions remains a great challenge and has technological application in a wide variety of areas, including the pharmaceutical, food, coatings, and building industries. Yield stress is a well-known but not understood property of many fluids, including cement-based materials (cement paste, mortars, and concrete). It is often thought of as the maximum force needed to break bonds in colloidal materials. However, analysis of the simulation data of dense suspension has shown that an important cause of yield stress is a supplementary stress that develops at the onset of flow. This supplementary stress is due to the organization of the contacts of aggregates in the compression quadrant, as stress is distributed throughout the suspension when it is sheared, and it is not accounted for by the simple breaking of bonds assumed in most theories of yield stress. This important discovery should affect how admixture companies design their products to mitigate this effect and reduce energy costs. William George is leading a group of researchers from the National Institute of Standards and Technology in using a computational approach for this research that is based on a modified Dissipative Particle Dynamics (DPD) model, which includes lubrication and Van der Waals forces for different-shaped particles near contact.

INCITE Allocation: 750,000 processor hours (IBM Blue Gene/P at ANL)

"The improved general understanding of rheological properties derived from this research should have a broad impact with results transferable to other complex fluid systems of interest such as nanoparticle systems."

—William George, National Institute of Standards and Technology

An Integrated Approach to the Rational Design of Chemical Catalysts

Catalysts feature prominently in cleaner and more efficient energy production, exemplified by fuel cell and other energy storage technologies. A deep understanding of the factors that determine the structure, energetics, and dynamics of molecules will be revolutionary, and will enable the rational design of chemicals, materials, and nanoscale

devices. The impacts of these breakthroughs are difficult to overestimate, yet they will not be realized without the assistance of a new generation of computational tools that are capable of providing truly reliable results for large molecular systems.

The INCITE-scale allocations on leadership computer systems are enabling the team led by Robert Harrison of ORNL to cross critical thresholds in the size and fidelity of our simulations. Also essential is the development of a new generation of tools that are capable of taking advantage of these new computers. Together, these advances in theory, software and hardware and software will enable a paradigm shift in how scientists use simulations because of the dramatic increase in the reliability of the computations and the size of the systems which may be studied. In the past year simulations have covered a wide range of physical systems, many closely coordinated with experimental studies. A novel hybrid method, developed by the team, allows for efficient inclusion of explicit solvent and was applied to study copper binding to prion protein (PrP). This protein is responsible for a group of neurodegenerative diseases called the transmissible spongiform encephalopathies, and the findings support the hypothesis that PrP acts as a copper buffer in vivo, protecting other proteins from the attachment of copper ions. Lignin is an excellent carbon-neural fuel and a potential alternative source of oxygenated chemicals and natural adsorbents. Femto- and even atto-second spectroscopy are now providing data at timescales pertinent to bond-breaking and even spectroscopic transitions. In preparation for simulations on systems of direct chemical significance that will require petascale computers the team is now using MADNESS to study the dynamics of few-electron systems in experimentally accessible laser pulses.

INCITE Allocation: 10,000,000 processor hours (Cray XT4. OLCF)

Development and Correlations of Larg-Scale Computational Tools for Flight Vehicles

The project led by Moeljo Hong of The Boeing Company is devoted to the development, correlations, and validations of large-scale computational tools for flight vehicles, thereby demonstrating the applicability and predictive accuracy of CFD tools in real-life production environment. One experiment within this project is to investigate the unsteady effects of a wing undergoes oscillations coupled with dynamic response from the wing structure. This ground breaking simulations requires coupling of two complex codes together in a nonlinear fashion: one for the aerodynamics, and one for the structural response of the wing. Such work helps validate our aeroelastic analysis processes before deployment for production use. The project will also be used to investigate a multidisciplinary design and optimization process of a wing strut and nacelle intersection region (for drag minimization) as well as exploration and validation of an unstructured-grid based process for high-lift analyses.

INCITE Allocation: 100,000 processor-hours (Cray XT4 OLCF), 300,000 hours (Cray X1E, OLCF)

“Boeing relies on partnerships such as INCITE to be able to access these computers in order to do proof-of-concept development and validation.”

–Moeljo Hong, The Boeing Company

Simulating the Quenching of Turbulent Flames by Fine Water Droplets
This INCITE project, led by Hong Im of the University of Michigan, utilizes terascale high-fidelity simulation capabilities to explore fundamental characteristics of nonpremixed flames in the presence of turbulent mixing and water spray injection. High performance computing has proven to be extremely effective for studying combustion chemistry to learn how mixing fuel and oxygen can be manipulated to change the burning process. In particular, this study ran simulations at NERSC seeking to explain how the interaction of water spray affects the chemistry and structure of the flame. Gaining a better understanding of these conditions may lead to improvements in fire suppression systems. Through the project, researchers determined a better method for describing the characteristics of spray-flame interactions. They then proposed a unified extinction criterion under which the spray would extinguish the flame, and tested this criterion on the large-scale simulation data produced under the project. The results demonstrated that the new extinction criterion serves as an objective and quantitative metric for the level of flame weakening arising from various physical mechanisms, thereby providing a convenient diagnostic tool for fire safety applications.

The computational model incorporates advanced submodels of soot formation, gray-gas radiation and lagrangian spray particle dynamics, all of which were developed through the ongoing university collaborative project supported by the DOE SciDAC program. The scientific objective is to understand the characteristics of flame suppression and extinction due to the interaction of turbulence, spray, chemistry and radiative heat transfer.

INCITE Allocation: 307,692 hours (NERSC HPC at LBNL)

High Power Electromagnetic Wave Heating in the ITER Burning Plasma
The next step toward fusion as a practical energy source is to develop a device capable of producing and controlling the high performance plasma required for self-sustaining fusion reactions, i.e., "burning" plasma. High-power electromagnetic waves in the radio frequency (RF) range have great potential to heat fusion plasmas into the burning regime, and to control plasma behavior through localized energy deposition, driven current, and driven plasma flows. This project extended wave-plasma interaction research conducted in the Scientific Discovery through Advanced Computing (SciDAC) program to the burning plasma regime of the International Tokamak Experimental Reactor (ITER). The extension to ITER is difficult because the physical size of ITER and the high plasma density require an order of magnitude increase in resolution over previous calculations. If successful, ITER could one day provide the world with a cleaner, more abundant energy source that produces no emissions and greatly reduces nuclear storage and proliferation. These simulations used 22,500 processor cores on the NCCS’s Jaguar to achieve 73 trillion calculations per second.

INCITE Allocation: 1,000,000 processor hours (Cray XT4. OLCF)

"We need to know which types of waves are present because different waves can interact differently with the plasma."

–Fred Jaeger, Oak Ridge National Laboratory

Understanding the electronic structure of novel electronic materials

Two important, and at first glance disparate, theoretical challenges in the understanding of modern electronic materials are: (1) Understanding the interface between an organic material and an inorganic conductor or semiconductor and its relation to transport of charge carriers across the interface, and (2) the electronic structure of novel magnetic materials and its relation to the mechanisms that control magnetism in such materials. Gaining a better understanding of these properties is not only of basic scientific interest, but could ultimately lead to improvements in technological areas such as spintronics, organic electronics, etc.

The most common approach for studying these problems is using density functional theory, or DFT. Unfortunately, further theoretical progress based on the DFT framework is hampered by two limitations of currently available DFT: the need to describe localized and delocalized electronic orbitals on the same footing, and the need to consider filled and empty electronic states equally. Here, we attempt to overcome these difficulties by turning to many-body perturbation theory for computing quasi-particle excitation energies. Our calculations are already shedding light on the electronic structure at the prototypical alkyl-chain/Si interface and we plan to build on this success to explore other systems of general interest.

INCITE Allocation: 124,615 Processor Hours (NERSC HPC)

"Many-body perturbation theory studies of large-scale systems are very intensive computationally. Our work would not have been possible without the high-performance 'franklin' machine at NERSC."

--Leeor Kronik, Weizmann Institute of Science

Illuminating Scientists' Knowledge of the Universe with "Standard Candles"

Led by Donald Lamb, ASC/Alliance Flash Center, University of Chicago, researchers are studying critical aspects of Type Ia supernovae, among the brightest and most powerful exploding stars in the universe. Type Ia create many of the elements from which we are made and are important for measuring distances in the universe. Two major challenges currently face Type Ia—1) buoyancy-driven turbulent nuclear burning, a key physical process in Type Ia, is not fully understood; and 2) few simulations of the four current models of Type Ia have been done. Working together, the researchers have optimized the FLASH code to run efficiently on all 163,840 processors of the IBM Blue Gene/P supercomputer at the Argonne Leadership Computing Facility for buoyancy-driven turbulent nuclear burning simulations. They have run a grid of simulations for different physical conditions. The researchers also have developed parallel processing tools needed to analyze the large amounts of data produced by the FLASH simulations. Preliminary analysis of these results shows that the flame surface is complex at large scales and smooth at small scales. The results of this work will be used to treat buoyancy-driven

turbulent nuclear burning more accurately in the whole-star, three-dimensional simulations of Type Ia at the NNSA ASC/Alliance Flash Center at The University of Chicago.

INCITE Allocation: 21 million processor hours (IBM Blue Gene/P at ANL)

"Buoyancy-driven turbulent nuclear burning is a key physical process in Type Ia, but we do not fully understand it. The computational resources awarded to the FLASH Center under the INCITE program allow us to carry out large, three-dimensional, multi-scale, multi-physics simulations to determine the nature of this process."

—Donald Lamb, ASC/Alliance Flash Center, The University of Chicago

Enabling Breakthrough Innovation at P&G

Some of the world's most well-known and highly regarded industrial companies have sought out Argonne's computing capability and technical expertise to convert that knowledge into transformative products and technologies. Procter & Gamble (P&G), one of the 25 largest U.S. companies by revenue, is among them. P&G researchers are using the Blue Gene/P system at the Argonne Leadership Computing Facility to investigate the molecular mechanisms of bubble formation in foams. Their U.S. Department of Energy INCITE allocation allowed them to perform computer simulations at an unprecedented scale on the dissolving of soap and foaming of suds. The researchers have developed coarse-grained models for two relevant surfactants. Ultimately, the work is expected to help P&G 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.

INCITE Allocation: 4 million processor hours (IBM Blue Gene/P at ANL)

"We wouldn't be able to conduct a computational experiment of this size without our partnership with Argonne. Already through this research, we have experienced a dramatically exciting new approach to evaluate materials. Fully matured, these methods could be used, for example, to evaluate bio-based replacements for petroleum-based ingredients—even guiding their development more effectively. Clearly, these learnings can be applied at P&G, but also extended to other wide-ranging uses outside the company, including formulations for other foam-based materials—even fire control chemicals."

—Tom Lange, Procter & Gamble

Petascale Computing for Terascale Particle Accelerator: ILC Design and Modeling

The International Linear Collider (ILC), a proposed electron-positron accelerator with an estimated cost of $6.75 billion, aims to elucidate the fundamental nature of matter, energy, space, and time. The ILC consists of two main linear accelerators (linacs), each 14 km in length, for producing electron and positron beams with 250 GeV energies. This INCITE project led by Lie-Quan Lee of the SLAC National Accelerator Laboratory will simulate the radio frequency unit and the basic accelerator section in the ILC main linacs and evaluate the effects of wakefields and heat loads. The simulations will play an

important role in ILC design, improving performance, increasing reliability, and lowering cost.

The existence of trapped modes in multi-cavity cryomodules or superstructures is a serious concern as they may pose deleterious effects on beam stability and generate unacceptable cryogenic loss. Systematic search for these dangerous modes in the cryomodule and RF (radio frequency) unit requires a huge amount of simulation effort. INCITE simulations in 2008 continued 2007 studies on the wakefield effects on an eight-cavity ILC cryomodule. A trapped module at 2.948 GHz, for example, was identified and found to have limited local heating, but trapped modes near 3.85 GHz were also identified, with local heating effects still needing to be investigated.

INCITE Allocation: 4,500,000 processor hours (Cray XT4. OLCF)

Tap It and Trap It: Investigation Underground Sequestration of CO_2

A team of researchers led by Peter Lichtner of Los Alamos National Laboratory (LANL) used the NCCS's Jaguar supercomputer to simulate carbon sequestration, searching for ways to maximize the benefits and avoid potential drawbacks. Using Jaguar, the team has been able to conduct the largest groundwater simulations ever seen, pursuing its research with a 2008 DOE/Office of Advanced Scientific Computing Research Joule metric code known as PFLOTRAN. The process simulated by Lichtner's team involves taking CO_2 that has been separated from a power plant's emissions and injecting it nearby into a deep saline aquifer one to two kilometers below the surface. The team investigated a process known as fingering that speeds the rate at which the CO_2 dissolves. Fingering grows out of the fact that while CO_2 in the supercritical phase is lighter than the surrounding brine, brine in which CO_2 has been dissolved is actually heavier than unsaturated brine. The result is a convection current, with fingers of the heavier, saturated brine sinking. This fingering in turn increases the surface area between the CO_2 and the brine and speeds the dissolution of the supercritical CO_2 into the brine. The simulations by Lichtner's team probed what happened to the CO_2 when injected into a deep saline aquifer, where it had to displace the brine that was present. Another goal of this project was to capture the observed slow leaching of uranium from the Hanford sediment and model the behavior of the uranium plume over time, taking into account variations in the Columbia River stage.

INCITE Allocation: 1,800,000 processor hours (Cray XT4. OLCF)

Assessing Global Climate Response of the NCAR-CCSM3: CO_2 Sensitivity and Abrupt Climate Change

The primary goal of this project was to perform the first synchronously coupled transient ocean/atmosphere/dynamic vegetation general circulation model simulation of the past 21,000 years using the NCAR Community Climate System Model (CCSM3). This experiment led by Zhengyu Liu, University of Wisconsin – Madison, addressed two fundamental questions on future climate changes: "What is the sensitivity of the climate system to the change of greenhouse gases, notably CO_2?" and "How does the climate system exhibit abrupt changes on decadal-centennial time scales?" Through their use of NCCS resources and CCSM3, the team is able to simulate many major features of the

deglaciation climate evolution and abrupt climate changes. Most notably, the Heinrich 1 (H1) event, the Bølling-Allerød (BA) warming, and the associated changes of the Atlantic thermohaline circulation are replicated in the simulation. The numerical results suggest that the abrupt climate change towards the BA is induced by the rebounding of the thermohaline circulation and the associated high latitude climate feedbacks in response to the demise of the North Atlantic meltwater forcing. This is in contrast to other theories involving hysteresis of the thermohaline circulation.

INCITE Allocation: 420,000 hours (Cray X1E, OLCF)

Multidimensional Simulations of Core Collapse Supernovae
This project performed 3-D simulations to understand how stars more than ten times the mass of our sun die in catastrophic stellar explosions known as core collapse supernovae. These events are the dominant source of elements in the Universe, including all the elements between oxygen and iron and half the elements heavier than iron; life would not exist without these elements. These supernovae are complex, 3-D, multi-physics events, but presently there are no 3-D models of sufficient realism, representing a significant void in supernova theory. These simulations were the first 3-D simulations performed with multifrequency neutrino transport, critical to realistic modeling of the neutrino shock reheating that is believed to be central to the supernova explosion mechanism. A complete understanding of the core collapse supernova mechanism requires parallel simulations in one, two, and three spatial dimensions. The nuclei in the stellar core undergo a transition through a series of complex shapes that can only be modeled only in three spatial dimensions. These modeling efforts will extend to three dimensions both the macroscopic and microscopic models of stellar core phenomena in core collapse supernovae.

INCITE Allocation: 6,000,000 processor hours (Cray XT4. OLCF)

“In a nutshell, this rapid advance in supercomputing technology will give us the tools to understand these events and their role in our universe,” Mezzacappa explained. “This is a very, very exciting and very satisfying thing.”

–Anthony Mezzacappa, Oak Ridge National Laboratory

BG/P Plan 9 Measurements on Large-Scale Systems
A team of researchers is working to provide a new software environment for supercomputers that makes the supercomputer appear to be part of the user’s desktop system, instead of a remote and hard-to-access external computer. Initial work is expanding the version of Plan 9 that was ported onto the BG/L system for the FASTOS program by Sandia National Laboratories, Bell Labs, IBM, and Vita Nuova. Led by Ronald Minnich, Sandia National Laboratories, the researchers are testing all aspects of the Plan 9 environment and modifying it as needed for large-scale machines.

INCITE Allocation: 1 million processor hours (IBM Blue Gene/P at ANL)

"Because the Plan 9 operating system was built with networks in mind, it requires less system administration support than other operating systems. In Plan 9's environment, files and directory trees can be imported from other machines, and with all resources defined as files or directory trees, sharing resources is greatly simplified. New drivers being tested will make it possible for native file systems to use, for example, the tree reduction network to make file systems very efficient."

—Ronald Minnich, Sandia National Laboratories

Molecular Simulation of Complex Chemical Systems

Understanding reactions on a molecular scale is critical to solving many of the challenges facing the 21st century. Leadership class computing provides scientists with the computational molecular simulations of reactions that will lead to unprecedented discovery and will move the field of molecular simulation to a radically new simulation protocol. Led by Christopher Mundy, researchers at Pacific Northwest National Laboratory, in collaboration with IBM Research, are applying statistical mechanical sampling methods in conjunction with density functional theory (DFT)-based interaction potentials to make detailed models of chemical processes at interfaces. The basic chemical physics of these leadership calculations will provide a detailed, molecular-scale picture of ions and reactions near interfaces. The researchers have obtained results on the free energies of transfer of OH^- and SO_2 from the bulk to interface. Through the direct simultaneous sampling of different reaction's coordinates, a picture is emerging where the structure and chemistry of species at interfaces differ dramatically from the bulk.

INCITE Allocations: 1.5 million processor hours (Blue Gene/P at ANL: 750,000; Cray XT4 at ORNL: 750,000)

"The use of leadership computing resources in conjunction with fast electronic structure algorithms has been critical to the correct statistical mechanical sampling on the systems of adequate spatial dimensions. INCITE resources are enabling us to take quantity (system size and number of CPUs) to a new quality (elucidation of chemical process in heterogeneous environments). These unique calculations contribute directly to DOE's Molecular Theory and Modeling Program, funded by Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences."

—Christopher Mundy, Pacific Northwest National Laboratory

Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean

A team led by Synte Peacock of the University of Chicago used the immense computing power at the National Center for Computational Sciences (NCCS) to run the most fine-grained, global-scale simulations ever of how the world's ocean regulate climate as a repository of greenhouse gases. In doing so, the team cast light on the currents and processes at work in the oceans as well as the possible fate of chemicals and gases – including carbon dioxide and other greenhouse gases – released into oceans. The team used the NCCS's Cray XT4 Jaguar supercomputer to perform the first-ever 100-year simulation of the ocean at a fine enough scale to include the relatively small, circular currents known as eddies. The inclusion of ocean eddies was a key element in the project. Ranging in diameter from about 60 miles near the equator to about 6 miles near the poles,

eddies play a key role in the dynamics of the ocean. Nevertheless, until recently researchers lacked the computing power to directly simulate eddies on a global scale.

INCITE Allocation: 3,163,000 processor hours (Cray XT4. OLCF)

"Half of the carbon dioxide that has been emitted over the last 100 years or so currently resides in the atmosphere. The rest is in the ocean."
– Synte Peacock, ASC/Alliance Flash Center, University of Chicago

Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences
This research team led by Michael Pindzola of Auburn University will apply state-of-the-art atomic and molecular collision codes to implement time-dependent simulations relevant for numerous applications, including ultra-short laser interactions with matter, plasma diagnostics in controlled fusion experiments, X-ray astronomy, synchrotron light sources, and free-electron lasers.

INCITE Allocation: 2,000,000 hours (Cray X1E, OLCF)

Modeling heliospheric phenomena with an adaptive, MHD-Boltzmann code
The solar system, tucked inside a bubble created by the continuous stream of charged particles being emitted by the sun, is drifting through a thin cloud of gas that permeates our neighborhood of the galaxy. This project uses a carefully crafted combination of computational techniques to examine the bubble (known as the heliosphere) as it interacts with the cloud (known as the Local Interstellar Medium), focusing on changes in the relationship throughout the sun's 11-year activity cycle. One goal is an analysis of the solar wind plasma (a stream of charged particles ejected from the upper atmosphere of the sun) interaction with partially ionized local interstellar medium (the gas and dust in space between stars in a galaxy) with a unique, multi-scale, continuum-kinetic approach and to evaluate the dependence of heavy galactic cosmic ray ion fluxes on the solar wind conditions in the heliosphere, which is key to planning future manned space missions to other planets.

This project was able to create an all-sky map of energetic neutral particles for the realistic orientation of the interstellar magnetic field to compare against the controversial observation of the STEREO (solar terrestrial relations laboratory) mission, which discovered considerable increases in energetic neutron atom fluxes. The work done is useful for the interpretation of NASA space missions, such as, STEREO, Voyager, and Ulysses.

INCITE Allocation: 850,000 processor hours (Cray XT4. OLCF)

"We have very complicated physics, where the transport of neutral particles should be modeled kinetically, the solar wind is magnetized in a complicated way, and multiple time scales participate in the problem. On the other hand, if we want to solve the SW-LISM interaction problem with realistic boundary conditions, we must have leadership

computer resources to propagate 1-day averaged data at Earth's orbit into the heliosheath beyond the termination shock, where plasma and energetic particle properties are measured by the Voyager spacecraft. Since the boundary conditions are very complicated and include transient phenomena of different length and time scale, only exceptionally fast (petascale) computers are capable of managing this problem."

–Nikolai Pogorelov, University of California, Riverside

Simulating Combustion in Gas Turbines

Researchers from the European Center for Research and Advanced Training in Scientific Computation (CERFACS) are developing and applying the Large Eddy Simulation (LES) Computational Fluid Dynamics (CFD) approach for the simulation of unsteady reacting flows. Led by Thierry Poinsot, they are focusing on technically challenging issues in real gas turbines, thereby demonstrating the usefulness of LES in the design process. These issues, which are beyond the capacities of currently used CFD tools, include ignition, reignition, flame quenching, and instabilities. While CFD research is often limited to a single burner, combining LES and the massively parallel computer resources at the Argonne Leadership Computing Facility allows the researchers to investigate the interaction of multiple burners in annular chambers and study important physical mechanisms, such as burner interactions, azimuthal acoustic modes generation, flame propagation from one burner to its neighbors, or how quenching occurs. Data gathered from this research will have real-world application in energy production (e.g., helicopter and aircraft engines).

INCITE Allocation: 4 million processor hours (IBM Blue Gene/P at ANL)

"The simulations performed to date would have taken over a year to perform on our current accessible computers. Also, parametric studies are impractical because having four or more simulations running for a year is not possible. Access to INCITE computers has allowed both. We have been able to demonstrate the important aspects of combustion instabilities, ascertaining predictions, and confirm what we found via experiments. This validates the whole computational approach applied in our preliminary full gas turbine simulations."

—Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation (CERFACS)

Optimizing the Beam Delivery System for X-Ray Free Electron Lasers

Using their INCITE 2008 allocation at NERSC, a team of accelerator researchers led by Ji Qiang at Lawrence Berkeley National Laboratory have identified key numerical parameters needed for accurate modeling of electron beam transport through an accelerator delivery system for an array of free-electron-laser based X-ray light sources. Such a high quality electron beam can be used for generating tunable coherent, ultra-fast, high brightness, intensive soft X-ray radiation for scientific discoveries in biology, material science, chemistry, and physics. By using supercomputers, researchers can develop, test and modify potential accelerator designs, saving both time and money in developing and building accelerators.

The team optimized the design of the beam delivery system towards using a single bunch compressor system and superconducting linear accelerator. The team found some optimal initial electron beam conditions that result in the best beam quality at the end of the delivery system. To accomplish this, they carried out the largest scale beam dynamics simulation in the accelerator community to date, based on multiple billion self-consistent macroparticle tracking. Using such a large-scale simulation, we have demonstrated that a good beam quality at 2.4 GeV with high peak current (~1 kA), small energy spread (~10^{-5}) and emittance (~1 mm-mrad) could be achieved through the optimized electron beam delivery system.

INCITE Allocation: 769,231 processor hours (NERSC HPC at LBNL)

"As we design next generation accelerators, high performance computing is essential for testing and validating ideas. The INCITE program provides unique, powerful computing resources for high precision optimization of beam delivery systems for future X-ray light source applications."

--Ji Qiang, Lawrence Berkeley National Laboratory

New Model Focuses on Effects of Clouds on Global Climate

To understand and predict climate change, it is critically important to represent the effects of cloud processes on the Earth's radiation budget and the distribution of precipitation. Our project involves directly simulating the global distribution of cloudiness using a "geodesic" grid that includes roughly a hundred million grid columns, each with 128 levels. The attached figure gives an idea of the shape of the geodesic grid; our model actually uses a much finer version of the grid with about ten thousand times more grid columns than shown in the picture. Using INCITE resources, we have successfully scaled the model out to 20,000 processors on Franklin, a Cray XT4 at the Lawrence Berkeley National Laboratory. During the coming year, we expect to demonstrate scaling to 80,000 or more processors.

INCITE Allocation: 153,846 processor hours (NERSC HPC at LBNL)

"INCITE is making it possible for us to represent the cloud processes of the climate system in more detail and with greater accuracy than ever before."

—David Randall, National Center for Atmospheric Research

Exploring New Concepts in Fusion Energy: Fast Ignition

Using their INCITE award at NERSC, fusion researchers led by Chuang Ren of the University of Rochester have been able to explore the feasibility of a new inertial confinement fusion concept: fast ignition. The ultimate goal of this research is to realize fusion as a controllable energy source and help solve the energy crisis facing the world today. In 2008, their simulations have shown that laser channeling can reduce the energy loss of an ignition pulse in the corona of a fuel pellet. The simulations have also shown that ultra-intense ignition pulses have an unexpectedly high efficiency in converting their energy to a form useful for ignition. These results will provide guidance for upcoming

fast ignition experiments on the new OMEGA-EP laser facility at the Laboratory for Laser Energetics at the University of Rochester and elsewhere.

INCITE Allocation: 307,692 hours (NERSC HPC at LBNL)

"These simulations model complicated physics and require extremely intense computation, which can only be accomplished with our INCITE grant."
Chuang Ren, University of Rochester

Quantum Spin Doctors Dissect Exotic States of Matter: Shedding Light on Bose Glass

Simulations performed by a team led by Tommaso Roscilde of France's École Normale Supérieure de Lyon and recently of Germany's Max-Planck Institute used the NCCS's Cray XT4 Jaguar supercomputer to explore the quantum mechanical phenomena that give us superconductors and superfluids. Roscilde and his teammates used Jaguar to simulate a lattice of atoms in a quantum magnet to examine two extraordinary quantum phases, or states of matter. In the first, called Bose-Einstein condensation, atoms throughout the material occupy the same state, with the same momentum, range of probable locations, and spin. In a quantum system, this is the closest they can get to being in the same place at the same time. By introducing impurities into the material, the team was also able to create the second phase, known as Bose glass. In a Bose glass, the impurities force the condensation into separate islands throughout the lattice, with atoms sharing the same state only with other nearby atoms. Roscilde's team is using a technique called Quantum Monte Carlo to simulate disorder in a quantum magnet and thereby create Bose glass. The team hopes its efforts will allow its collaborators—Vivien Zapf and Marcelo Jaime at the National High Magnetic Field Laboratory at Los Alamos National Laboratory—to perform the first experimental confirmation of Bose glass. This work is at the cutting edge of condensed-matter science.

INCITE Allocation: 1,200,000 processor hours (Cray XT4. OLCF)

"I find that in this particular instance of a study of a solid-state system, you're really trying to tailor matter to a level of control that was unthinkable a few decades ago or even a few years ago. What you have is a system where, in principle, you can tune the system among completely exotic phases that have no analog in classical systems."
–Tommaso Roscilde, École Normale Supérieure de Lyon

Breaking New Ground in Membrane Protein Research

Numerous biological processes are controlled by proteins in the cell membrane, ranging from production of biofuels to cleaning up toxic organic waste. Large-scale gating motions, occurring on a relatively slow time scale, are essential for the function of many important membrane proteins such as transporters and channels. Voltage-activated ion channels are literally electric switches that are turned "on" by a change in the cellular potential. Malfunction of those channels can lead to cardiac arrhythmia and neurological pathologies. Led by Benoit Roux, Argonne National Laboratory and The University of Chicago, in collaboration with researchers from the University of Illinois, Urbana-

Champaign, the research team used high-performance computing to break new ground in understanding how these membrane proteins work. Exploiting state-of-the-art developments in molecular dynamics and protein modeling, the team constructed models of voltage-gated potassium channels and ran them on Argonne National Laboratory's Blue Gene/P and Oak Ridge National Laboratory's Cray XT leadership-class computers, using INCITE resources. An important result of these simulations concerns the properties of the electric field responsible for the voltage activation. The calculations show that this electric field is indeed more intense than at other equivalent positions across the membrane far away from the protein. These results open up the possibility of better-designed therapeutic drugs, as well as the construction of artificial biomemetic nano-switches.

INCITE Allocations: 5 million processor hours (IBM Blue Gene/P at ANL: 1.5 million; Cray XT4 at ORNL: 3.5 million)

"Being able to run on these top computers is essential for this work. The time and energy scales of the underlying molecular processes are just within reach of the computational capabilities of such leadership-class computers."

—Benoit Roux, Argonne National Laboratory and The University of Chicago

Predictive and Accurate Monte Carlo Based Simulations for Mott Insulators, Cuprate Superconductors and Nanoscale Systems.

Working from fundamental principles of quantum mechanics, a team of materials scientists led by Jorge Sofo of Penn State University and Thomas Schulthess of ORNL used Jaguar to accurately simulate the behavior of water in the presence of the common catalyst titanium dioxide. The work not only improves our understanding of a process that is already important in areas such as fuel cells and the geosciences; it also prepares the way for simulations of ever more complex systems. Specifically, the team simulated the process by which water passes protons from one molecule to another. While a molecule of water—H2O—contains two hydrogen atoms and one oxygen atom, one of the hydrogens will occasionally break off. The nucleus of this hydrogen—a proton—can then be exchanged with other hydrogens in other water molecules, transporting the proton through the water. The simulation shows that first- principles molecular dynamics—in this case performed using the Vienna Ab-Initio Simulation Package—can be used to explore this process. The computer specialists were able to compare their results with results from a team of experimentalists led by Dave Wesolowski of ORNL, which evaluated the same system of water and titanium dioxide molecules using neutron-scattering techniques.

The team received the prestigious 2008 Association for Computing Machinery (ACM) Gordon Bell Prize at the SC08 supercomputing conference after attaining the fastest performance ever in a scientific supercomputing application.

Schulthess, along with Thomas Maier, Michael Summers and Gonzalo Alvarez, all of ORNL, achieved 1.352 quadrillion calculations a second—or 1.352 petaflops—on ORNL's Cray XT Jaguar supercomputer.

INCITE Allocation: 10,000,000 processor hours (Cray XT4. OLCF)

"This whole simulation sets the stage for a lot more work on more complicated systems. This is much more than a proof of concept because we've got a lot of science out of this, but the idea is obviously to move on to more complicated materials."

–Paul Kent, Oak Ridge National Laboratory

Predicting Thermal Striping in Sodium-Cooled Reactors

Computer simulation is aiding the design optimization of a new generation of Advanced Recycling Reactors (ARR). These reactors will be used to greatly reduce the amount of spent fuel storage required by light water reactors. A critical issue in the design of sodium-cooled fast reactors is predicting the phenomenon of "thermal striping"—when partially mixed streams of sodium coolant expose structural materials to cyclic thermal stresses that cause fatigue and limit their lifetime. Traditionally, designers have relied on data from instrumented experiments, but this data is expensive and difficult to collect and greatly limited in its spatial fidelity and adaptability to scope design space. Led by Andrew Siegel, Argonne National Laboratory researchers are using INCITE resources to carry out the first detailed numerical experiments of thermal striping on realistic reactor geometries.

INCITE Allocation: 5 million processor hours (IBM Blue Gene/P at ANL)

"The results of our research can be directly used by U.S. ARR designers to create a more optimized design."

—Andrew Siegel, Argonne National Laboratory

Breaking Down the Plant Walls to Advance Biofuels Research

Efficient production of ethanol via hydrolysis of cellulose into sugars is a major energy policy goal. This project performed highly parallelized multi-length-scale computer simulations to help understand the physical causes of resistance of plant cell walls to hydrolysis—the major technological challenge to developing cellulosic bioethanol. Plant cell wall lignocellulosic biomass is a complex material composed of crystalline cellulose microfibrils laminated with hemicellulose, pectin, and lignin polymers. The simulations are part of a larger effort to integrate the power of neutron scattering and high-performance computing at Oak Ridge National Laboratory to derive information about lignocellulosic degradation that is unprecedented in detail.

"Understanding the mechanism by which proteins fold up into unique 3-D architectures is a holy grail in molecular biology."

– Jeremy Smith, Oak Ridge National Laboratory

INCITE Allocation: 3,500,000 processor hours (Cray XT4. OLCF)

Better Understanding the Interactions between Quarks and Gluons

Scientists are seeking to increase their knowledge of the interactions between quarks and gluons, the basic constituents of 99% of the visible matter in the universe. Their research

will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature. The scientists are generating gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to their physical values found in nature. The Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) has tremendously accelerated the generation of the gauge configurations—in many cases, by a factor of 5 to 10 over what has been possible with other machines. Significant progress has been made in simulations with two different implementations of quarks—domain wall and staggered. The work will greatly improve the accuracy of the scientists' determination of a wide range of important quantities in high energy and nuclear physics. The project is being undertaken by the USQCD Collaboration, which is comprised of nearly all of the high energy and nuclear physicists in the United States working on the numerical study of quantum chromodynamics, the theory of quarks and gluons.

INCITE Allocation: 26,700,000 processor hours (IBM Blue Gene/P at ANL: 19,600,000; Cray XT4 at ORNL: 7,100,000)

"The combination of Early Science Program and INCITE time made available at the ALCF over the past six months has advanced the study of chiral fermions and improved staggered quarks by nearly a year. We presented scaling results for neutral K meson mixing, quark masses, pseudo scalar decay constants, and nucleon form factors at Lattice 2008, which would otherwise have been unavailable until well into 2009."

—Bob Sugar and Norman Christ, USQCD Collaboration

Simulation Aids Development of First Coal Plants with Near-Zero Emission

DOE researchers at the National Energy Technology Laboratory (NETL) and ORNL used supercomputers to improve the industrial design of facilities that tap coal's oxidative potential while trapping its pollutants. The highest-resolution coal-gasification simulation to date will help enable faster development of clean coal technology that emits nearly no nitrogen oxide, mercury or sulfur and that sequesters most carbon dioxide. In gasification, coal is pulverized and partially oxidized to separate fuel-rich hydrocarbons from pollutants. Coal solids are recycled through the system until they are completely gasified to produce "syngas," a mixture of hydrogen and carbon monoxide. The syngas can be used to produce hydrogen or to generate electricity (for example, using gas turbines) in a clean and efficient manner. To examine injection ports in detail, the NETL researchers ran simulations on Jaguar for two weeks in January 2008 at 1 millimeter resolution. Jaguar's high resolution means combustion can be modeled in great detail, enabling simulations that represent reality with unprecedented fidelity. Jaguar's enormous memory and speed produced quicker answers to scientific and engineering questions and therefore will help to accelerate development of the technology.

INCITE Allocation: 3,000,000 processor hours (Cray XT4. OLCF)

“An important part of NETL’s mission is to supply clean coal technology, and our research group at NETL develops computational tools and applications in support of that mission.”

–Madhava Syamlal, National Energy Technology Laboratory

“Essentially, we’re trying to get the highest-resolution data to date for coal gasification to feed into these test facilities. Correctly capturing inlet regions is critical in our simulations, not only to understand local conditions in these areas, but also to understand how injection of coal can impact the conversion of coal into syngas.”

–Chris Guenther, National Energy Technology Laboratory

High-Resolution Global Simulation of Plasma Microturbulence

Use of predictive computational models derived from first-principles physics equations has allowed for unparalleled gains in scientists' knowledge of microturbulence. Led by William Tang of the Princeton Plasma Physics Laboratory (PPPL), scientists from PPPL, Columbia University, and Oak Ridge National Laboratory have significantly enhanced the capabilities of a 3-D global particle-in-cell code (GTC) by employing a hybrid (Open MP/MPI) approach which has enabled more effective utilization of the Argonne Leadership Computing Facility's (ALCF) Blue Gene/P quad-core LCF. The BG/P's multi-core system now allows higher-resolution simulations in a multi-dimensional phase-space for conducting a realistic examination of the effect of collisions on plasma confinement properties. With this unprecedented capability, advanced kinetic simulations with higher physics fidelity can be directly applied for the systematic interpretation of experimental results in the near future. This, in turn, will help pave the way for scientific discoveries needed for accelerating progress towards the ultimate goal of attaining and harnessing essentially inexhaustible fusion power in the form of a secure and reliable energy system that is environmentally and economically sustainable.

INCITE Allocation: 2 million processor hours (IBM Blue Gene/P at ANL)

“The INCITE award enabled systematic runs demonstrating the improved efficiency of the new hybrid approach (Open MP/MPI) implemented into GTC over that of the code run with MPI alone on BG/P. It has also supported the valuable developmental activities appropriate for the initial months of this new leadership class facility’s operation. These activities have positioned the project very well to move forward in FY2009 with production runs to capture the important information on ITER-scale plasmas with unprecedented resolution in a multi-dimensional phase-space to deliver scientific results appropriate for ‘path to petascale’ grand challenges.”

—William Tang, Princeton Plasma Physics Laboratory

Modeling the Molecular Basis of Parkinson’s Disease

As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson’s disease are enormous. Currently, there are more than 2 million cases in the United States. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone. University of California—San Diego scientists are leveraging the high-end computation power of the Blue Gene/P at the Argonne

Leadership Computing Facility to learn more about the molecular basis of the disease and explore ways to treat it. They have found that the clumping of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes. In contrast, another protein, beta-synuclein (bS), appears to block the clumping action. The findings provide a test bed for identifying possible therapeutic interventions through computational modeling. Given the encouraging correlation between their molecular dynamics modeling predictions and laboratory experimental results, the team expects to make steady progress both with the computational model itself, as well as with the design of effective drugs based on the computational modeling and simulations.

INCITE Allocation: 1.2 million processor hours (IBM Blue Gene/P at ANL)

"An anti-Parkinson's drug based on the results of our modeling and simulations is in the early stages of development. The intermediate pro-drug showed preliminary results of slowing aggregation of alpha-synuclein—the unstructured protein that has been shown as one of the main causes of Parkinson's disease. These studies are impossible without a high-performance computer, which is the Blue Gene at Argonne National Laboratory."
—Igor Tsigelny, University of California—San Diego/SDSC

Solar Cells at the Nanoscale: Can Tiny Materials Help Solve Big Energy Challenges?

A computer method created to understand the energy-harnessing potential of nanostructures for solar cell design utilized its INCITE award on ORNL's Jaguar supercomputer, as well as supercomputers at NERSC and Argonne National Laboratory, en route to winning a prestigious ACM Gordon Bell Prize for algorithm innovation at the SC08 conference. Led by LBNL's Lin-Wang Wang, the Linear Three Dimensional Fragment (LS3DF) method's initial runs on NERSC's Cray XT4 system provided key insights about the application that eventually led to the prize. According to Wang, nanostructures -- tiny materials 100,000 times finer than a human hair, may hold the key to energy independence. The team optimized their code at NERSC, with the code running on 17,280 cores of the original dual-core Franklin computer system. In one hour, team members calculated the electronic structure of a 3,500-atom ZnTeO alloy, verifying that the code could be used to compute properties of the ZnTeO alloy that previously had been experimentally observed. Once the LS3DF code had been optimized it was a matter of days before it was running at each of the DOE supercomputing facilities. At the Argonne Leadership Computing Facility, the code ran on 163,840 cores, on the IBM BlueGene/P system reaching 224 teraflop/s on or 40.5 percent of the system's peak performance capability. ORNL then invited Wang and other Gordon Bell finalists to carry out runs on ORNL's petaflop supercomputer, Jaguar, where the LS3DF application ultimately achieved a speed of 442 teraflop/s (442 trillion calculations per second) on the Cray XT5 system with 147,146 cores.

INCITE Allocation: 2,100,000 processor hours (Cray XT4. OLCF)

"To calculate the electronic structures of some nanosystems, large computing resources are needed. The INCITE award allocation allows us to finish many calculations in a few

hours on the largest supercomputers in the world, rather than weeks on the small computers. It also enables us to tackle scientific problems with realistic size scale and accuracy which would be impossible otherwise."

–Lin-Wang Wang, Lawrence Berkeley National Laboratory

Climate Science Computational End Station Development and Grand Challenge

Advanced computation, like that possible on the Blue Gene/P supercomputer at the Argonne Leadership Computing Facility (ALCF), allows researchers at the National Center for Atmospheric Research (NCAR) and U.S. Department of Energy (DOE) laboratories to develop more complex and intricate climate models. The vital information provided by these improved models will guide environmental policy. Using ALCF resources, the Climate Science Computational End Station is advancing climate science through both an aggressive model development activity and an extensive suite of climate simulations, particularly the correct simulation of the global carbon cycle and its feedback to the climate system. The NCAR and DOE researchers tested a new, highly scalable method for solving the fluid dynamics of the atmosphere. This atmospheric Community Climate System Model component, called CAM/HOMME, has been shown to run with a resolution as high as 1/8 of a degree of latitude on over 80,000 cores. The research is being led by Warren Washington, National Center for Atmospheric Research (NCAR), in collaboration with other researchers from NCAR, Argonne National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, NASA Headquarters, and Georgia Tech University.

INCITE Allocations: 18,026,000 processor hours (IBM Blue Gene/P at ANL: 1 million; NERSC HPC at LBNL: 1,308,000; Cray XT4 at ORNL: 15,718,000)

"The INCITE-supported development of a massively parallel Community Climate System Model is absolutely critical for climate scientists who will be carrying out the massive set of societal and policy-relevant simulations for the IPCC AR5. These simulations will require much higher model resolutions, using much more expensive biogeochemistry and atmospheric chemistry packages, which must run efficiently at scale on the next generation of massively parallel machines."

—Warren Washington, National Center for Atmospheric Research

Accelerating the Pace of Discovery in Alternative Fuels Research

Scientists continue to seek clean, renewable energy sources that will reduce our dependence on foreign oil. One promising possible energy source for cars is hydrogen. However, currently available methods of storing hydrogen in materials are typically either much too heavy or else bind the hydrogen within the material much too strongly. Quickly extracting hydrogen out of those materials requires extremely high levels of heat—impractical for actual use in vehicles on the open road. In research led by Christopher Wolverton at Northwestern University, in collaboration with the University of California—Los Angeles, researchers have recently developed a suite of computational materials science tools aimed at the discovery of novel hydrogen storage

materials. The suite is based on first-principles methods that start with a quantum-mechanical description of the interaction of electrons in a solid. Using the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF), the novel tools allow the prediction of the thermodynamic conditions under which hydrogen can be inserted and removed from a given material, while also predicting the new atomic-scale crystal structure of the predicted material. These capabilities have led to the prediction of several novel, high-density hydrogen storage materials and reactions.

INCITE Allocation: 1 million processor hours (Blue Gene/P at ANL)

"Our calculations require state-of-the-art, first-principles molecular dynamics simulations, using a very large system size (i.e., thousands of atoms) and a very long simulation time. The types of atomic-scale kinetic calculations we are undertaking are simply impossible without the large-scale computing resources generously made available through the Department of Energy's INCITE program."
—Christopher Wolverton, Northwestern University

First Principles Models of Type Ia Supernovae
This project studied four key stages of Type Ia supernovae, the largest thermonuclear explosions in the universe: the long-time convection that leads to ignition of the first flames; the propagation of these resultant flame(s) through the star leading to the explosion itself; and finally, the radiation-dominated phase at the end of the explosion. This is an especially relevant problem in astrophysics today: by acting as standard candles, Type Ia supernovae have been at the forefront of a revolution in modern cosmology, leading to the discovery that the expansion rate of the Universe is accelerating.

INCITE Allocation: 3,500,000 processor hours (Cray XT4. OLCF)

"We would like to understand the physics underneath. Type Ia supernovas are still one of the most important pieces of evidence for an accelerating expansion of the universe."
–Stan Woosley, University of California, Santa Cruz

Performance Evaluation and Analysis Consortium End Station
The Performance Evaluation and Analysis Consortium (PEAC) End Station provides the performance community with access to the U.S. Department of Energy's leadership class computing facilities (LCF). The performance community, in turn, supports the centers and the computational scientists conducting research at these centers in many ways: developing performance tools and other performance-related infrastructure, characterizing performance and providing guidance on using the systems, and working directly with important simulation models. Recent results include the initial port of the Berkeley UPC compiler to the Blue Gene/P (available for download at http://upc.lbl.gov/download). The PEAC's INCITE allocation was also used in the performance analysis and optimization of a code that won a special ACM Gordon Bell Prize for algorithm innovation, presented at SC08, and in a SC08 paper on evaluating the promise of the BG/P architecture for computational science. Patrick Worley, Oak Ridge National Laboratory, is leading a team of researchers from Lawrence Berkeley National

Laboratory, University of Tennessee, Argonne National Laboratory, University of Maryland, University of Oregon, Rice University, University of Wisconsin, University of North Carolina, University of California—San Diego, University of California—Berkeley, Oak Ridge National Laboratory, and Lawrence Livermore National Laboratory in the PEAC initiative.

INCITE Allocations: 8 million processor hours (Cray XT4 at ORNL: 4 million; Blue Gene/P at ANL: 4 million)

"The ultimate goal of the PEAC community is to improve the productivity of high performance computing centers and their users. Without access to LCF systems, such as those provided by the INCITE program, it would be impossible for us to achieve this goal."

—Patrick Worley, Oak Ridge National Laboratory

Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas

Predicting and controlling turbulent transport in fusion plasmas are among the most important and challenging scientific issues facing the International Thermonuclear Experimental Reactor (ITER) project. Nonlinear plasma dynamics and self-organization in complex tokamak geometry are exceedingly challenging, requiring multi-scale, nonlocal processes of turbulence. In this project, a research team led by Patrick Diamond of the University of California, San Diego employs nonlinear simulations using a gyrokinetic toroidal code (GTC) for tokamak core, and another gyrokinetic particle-in-cell code (XGC) for tokamak edge. They will validate the predictive capability of the GTC and XGC dynamical models by comparing simulation results with the largest fusion experiments in the United States (DIII-D, ALCATOR C-MOD, and NSTX tokamaks). This research will assist in the design and construction of ITER, a prototype fusion reactor to be built in France in 2018. If successful, ITER could one day provide the world with a cleaner, more abundant energy source that produces no emissions and greatly reduces nuclear storage and proliferation issues. In 2008 the team completed what is arguably the largest run in fusion simulation history, using 93 percent of the NCCS's flagship supercomputer Jaguar, a Cray XT4, with the classic fusion code GTC (Gyrokinetic Toroidal Code), the key production code of two fusion SciDAC projects (GPS-TTBP and GSEP). The researchers discovered, among other things, that for a device the size of ITER, the containment vessel would demonstrate GyroBohm scaling, meaning that the heat transport level is inversely proportional to the device size. In other words, the simulation supports the ITER design: a larger device will lead to more efficient confinement.

INCITE Allocation: 8,000,000 processor hours (Cray XT4. OLCF)

"The success of fusion research depends on good confinement of the burning plasma. This simulation size is the one closest to ITER in terms of practical parameters and proper electron physics."

–Yong Xiao, University of California, Irvine

Electronic, Lattice and Mechanical Properties of Novel Nano-Structured Bulk Materials

More than 60 percent of the energy created by a vehicle's engine is lost as waste heat, but thermoelectric materials promise to take that heat and turn it into electricity, saving potentially hundreds of millions of gallons of gasoline each year. This project by Jihui Yang of General Motors addressed a key issue in the study of superior thermoelectric materials, the role of nanostructural features in the electronic, lattice, and mechanical properties of nanostructured bulk materials. The NCCS's Jaguar made possible the GM team's largest-ever simulation, which examined a 1,000-plus atom supercell.

INCITE Allocation: 10,000,000 processor hours (Cray XT4. OLCF)

"Quantum mechanical ab initio calculations are usually done with 200 to 300 atoms. We're doing calculations with a unit cell of more than 1,000 atoms. People would not be able to dream of doing these calculations without a large computing facility."

–Jihui Yang, GM R&D Center