Type: New
Title: "Adaptive Detached Eddy Simulation of a Vertical Tail with Active Flow Control"

Principal Investigator: Kenneth Jansen, University of Colorado
Co-Investigators: Michel Rasquin, University of Colorado
Onkar Sahni, Renssalaer Polytechnic Institute
Mark Shephard, Renssalaer Polytechnic Institute
Philippe Spalart, The Boeing Company
Edward Whalen, The Boeing Company

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation: **40,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (40,000,000 processor hours)

Research Summary:
The use of fuel—and its accompanying costs—has become an increasing concern in many industries. Researchers are examining the issue of fuel reduction in commercial jet aircraft from the perspective of redesign. By redesigning the vertical tail of a commercial jet, they hope to reduce jet fuel use by 0.5%, resulting in annual savings of $300 million.

Using "synthetic" commercial jet aircraft, the team will perform a series of simulations of active flow control on the vertical tail of the aircraft. The team will model an array of jets that have been vectored to augment the streamwise momentum near the rudder suction peak, where separation is typically observed to limit rudder effectiveness. The simulations are carefully coordinated with an experimental effort funded under the same project.

As the experiments are at a much lower Reynolds number than those encountered in flight, the first set of detached eddy simulations (DES) are designed to be validated against the coordinated experiments, matching all details, including the complicated jet cavity paths. As it will not be possible to carry out this level of simulation at flight Reynolds numbers, this project will also validate a multiscale modeling effort that has been developed for this purpose. Simulations at each Reynolds number will be analyzed for insight into improving Reynolds averaged Navier-Stokes (RANS) modeling for this class of problems.

Currently, the vertical tail in jet aircraft is sized to handle an "engine-out" condition, which requires it to be much larger than what is needed for all other conditions. Researchers hypothesize that if flow control can achieve the same side force with a 25% smaller vertical tail, jet-fuel reduction will result.

Type: Renewal
Title: Advanced Reactor Thermal Hydraulic Modeling

Principal Investigator: Paul Fischer, Argonne National Laboratory
Co-Investigators: Elia Merzari, Argonne National Laboratory
Aleksandr Obabko, Argonne National Laboratory
W. David Pointer, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Nuclear Energy

INCITE Allocation: **25,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (25,000,000 processor hours)

Research Summary:
The DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing simulation capabilities to leverage U.S. leadership computing facilities in the design of next-generation nuclear reactors capable of providing sustainable energy with a low carbon footprint. One active area of research is the Advanced Fuel Cycle Initiative (AFCI), which is examining a closed nuclear fuel cycle based on a new generation of fast neutron reactors specifically designed for the transmutation of spent nuclear fuel to address nuclear waste management concerns. Partitioning and transmutation of transuranic elements from nuclear spent fuel is considered as a way of reducing the burden of geological disposal.

Advanced simulation is viewed as critical in bringing fast reactor technology to fruition in an economic and timely manner, and the DOE has recently established area-specific campaigns to look at open questions in closing the fuel cycle. Analysis of fast reactor cores is one of the areas of interest, and the thermal-hydraulic performance—pressure drop and mixing induced by the coolant flow—figures prominently in design questions.

In accordance with the original proposal, the team has already undertaken a series of computational studies of fluid and heat transfer flows aimed at the validation of LES Nek5000 high Reynolds-number capability for thermal hydraulics phenomena emerging in design and analysis of future generations of nuclear power plants. Since the focus of the team's NEAMS funding has been changed from sodium fast reactors to technology neutral analysis, 2012 research plans have also adjusted slightly. The team will finish its 37-pin rod bundle simulation with and without wire-up and move to the 25-pin study for the 2012 OECD/NEA benchmark problem (MATIS) for spacer grid analysis. Planned INCITE work for 2012 includes: 1) a comparative study of 37-pin rod bundles with wire wrap, bare rod, and spacer grids to contrast with the conducted study of a single pin in a periodic array; 2) 25-pin study for 2012 MATIS benchmark problem for spacer grid analysis. Between 500-1,000 million grid points and 15 million hours are estimated for the MATIS case.

Type: New
Title: "Atomistic Adaptive Ensemble Calculations of Eutectics of Molten Salt Mixtures"

Principal Investigator: Saivenkataraman Jayaraman, Sandia National Laboratories
Co-Investigators: Steve Plimpton, Sandia National Laboratories
Aidan Thompson, Sandia National Laboratories
O. Anatole von Lilienfeld, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Solar Energy

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
New and improved heat-transfer media with higher operating temperature ranges promise to turn solar-thermal power into a competitively cost-effective energy source. Molten salt mixtures are good candidates because of their high thermal decomposition temperatures. But their associated high boiling points are not an ideal property for solar-thermal energy production, which needs a large operating temperature window for optimal thermodynamic efficiency. The molten salt mixtures with the best eutectic balances need to be identified, but eutectic screening of multicomponent solutions has heretofore been cumbersome and time-consuming.

This project combines petascale high-performance computing with novel atomistic molecular dynamics simulations to efficiently predict the eutectic compositions in multi-component mixtures. The method exploits the interpolation of force fields ("alchemical" changes) in classical molecular dynamics within ensembles that communicate during the course of a single parallel run for locating the eutectic point of a given dimensionality of the mixture. The suitability of this scheme was demonstrated in a previous study at the Argonne Leadership Computing Facility by the authors for eutectic points of binary and ternary mixtures of lithium, sodium, and potassium nitrate mixtures.

The ability to rapidly predict the eutectics of multicomponent salt mixtures would make solar-thermal power facilities significantly more cost effective. It would also drastically reduce the costs for constructing solar-thermal power plants, because heated pipes that prevent crystallization of cold salts would not be needed if melting points could be lowered to ambient temperatures.

Type: Renewal
Title: "Cellulosic Ethanol: Simulation of Multicomponent Biomass System"

Principal Investigator: Jeremy Smith, Oak Ridge National Laboratory
Co-Investigators: Xiaolin Chang, Oak Ridge National Laboratory
Loukas Petridis, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **23,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (23,000,000 processor hours)

Research Summary:
Rational strategies for improving the efficiency of biofuel production from plant cell wall lignocellulosic biomass *via* cellulose hydrolysis require a detailed understanding of the structure and dynamics of the biomass. Lignocellulosic biomass is a complex material composed of cellulose microfibrils laminated with hemicellulose, pectin, and lignin polymers. To reduce biomass recalcitrance to hydrolysis by the improvement of pretreatment and the design of improved feedstock plants, a detailed understanding of biomass structure, mechanics, and response to pretreatment regimes is needed. During a previous INCITE award, we applied molecular dynamics (MD) simulation to understand the structure and dynamics of lignin aggregates and of lignin precipitation on celluslose fibers. During this time we also developed technology permitting the efficient simulation of multimillion atom biomolecular systems running on O(~10-100k) cores. This enables us to plan, for the present award, to extend the lengthscale of the systems under study to enable the simulation of full lignocellulosic biomass systems, consisting of cellulose, lignin and hemicelluloses, together in specific cases with hydrolyzing enzymes.

The research aims at providing simulation models of biomass and biomass:enzyme interactions that will help us understand the physical origins of biomass recalcitrance, using atomic-detail computer simulation of biomolecular systems with the molecular dynamics (MD) method involving the stepwise integration of the equations of motion. The detailed multiscale structure revealed by these simulations will aid in understanding biomass recalcitrance to hydrolysis and in engineering efforts to improve second-generation biofuel yield.

Type: Renewal
Title: "Climate-Science Computational Development Team: The Climate End Station II"

Principal Investigator: Warren Washington, University Corporation for Atmospheric Research

Co-Investigators: Philip Cameron-Smith, Lawrence Livermore National Laboratory
Scott Elliott, Los Alamos National Laboratory
David Erickson, Oak Ridge National Laboratory
Steven Ghan, Pacific Northwest National Laboratory
James Hack, Oak Ridge National Laboratory
Jim Hurrell, University Corporation for Atmospheric Research
Rob Jacob, Argonne National Laboratory
Philip Jones, Los Alamos National Laboratory
Jean-Francois Lamarque, University Corporation for Atmospheric Research
L. Ruby Leung, Pacific Northwest National Laboratory
Bette Otto-Bliesner, University Corporation for Atmospheric Research
Steven Pawson, NASA
Mark Taylor, Sandia National Laboratories
Peter Thornton, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **86,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (56,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (30,000,000 processor hours)

Research Summary:
The Climate Science Computational End Station (CCES) will predict future climates using scenarios of anthropogenic emissions and other changes resulting from energy policy options. CCES will also improve the scientific basis, accuracy, and fidelity of climate models, delivering climate change simulations that directly inform national science policy, thereby contributing to the DOE, NSF and NASA science missions. Of particular importance is the improved simulation of the global carbon cycle and its feedbacks to the climate system, including its variability and modulation by ocean and land ecosystems. Continuing model development and extensive testing of the CCSM system to include recent new knowledge about such processes is at the cutting edge of climate science research.

Type: Renewal
Title: "Coarse Grained Molecular Dynamics Studies of Vesicle Formation and Fusion"

Principal Investigator: Michael Klein, Temple University
Co-Investigators: Russell DeVane, Procter & Gamble
Peter Koenig, Procter & Gamble
Axel Kohlmeyer, Temple University
Vincenzo Carnevale, Temple University
Giacomo Fiorin, Temple University

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **18,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (18,000,000 processor hours)

Research Summary:
Membrane fusion, the process in which two lipid bilayers merge to form a continuous structure, is a complex and fascinating phenomenon, influenced by many factors including membrane composition, hydration, electrostatics, and environmental conditions. Membrane fusion is essential for the life cycle of all living organisms. In industrial processes, vesicle or membrane fusion is an undesirable event leading to largescale product instabilities. A number of formulated consumer products are made of dispersed vesicles which contain active components or are themselves active ingredients defining the product's performance.

A molecular view of the role of fusion proteins in the membrane fusion process is largely lacking and it is not likely that experiments alone can provide these details in the foreseeable future. To simulate these processes, accurate coarse-grain models, molecular dynamics software at the limit of its capabilities as well as exceptionally capable computer hardware are required. In preparation for this project, enhancements to the LAMMPS molecular dynamics package have been implemented. Future improvements to overall performance and scaling to large node counts will be realized, and these improvements are applicable to other projects using LAMMPS.

Type: New
Title: "Control of Complex Transformations with Advanced Molecular Simulation Methods"

Principal Investigator: Christopher Mundy, Pacific Northwest National Laboratory
Co-Investigators: Juerg Hutter, University of Zurich
Shawn Kathmann, Pacific Northwest National Laboratory
Simone Raugei, Pacific Northwest National Laboratory
Roger Rousseau, Pacific Northwest National Laboratory
Greg Schenter, Pacific Northwest National Laboratory
Bruce Palmer, Pacific Northwest National Laboratory
Joost Vandevondele, University of Zurich

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **12,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (12,000,000 processor hours)

Research Summary:
To advance our capabilities for the computational studies of chemical reactivity in complex environments there are two required ingredients: advanced sampling techniques (for accurate free energies) and efficiently going beyond gradient corrected density functional theory (DFT) in the condensed phase for more accurate description of electronic states. As outlined in a 2007 DOE Basic Energy Sciences workshop report *Basic Research Needs: Catalysis for Energy* these two theoretical approaches are singled out as high priority scientific challenges that are necessary for the accurate prediction of the chemical reactivity of complex catalytic materials.

By obtaining an accurate estimate of the free energy of thermal, electro or photocatalytic processes at finite temperatures it is envisioned that theory and computation will be able to take a leadership role in the development of new and efficient catalysts for the interconversion and control of chemical, electrical and solar energy that will lead to the future development of transformative energy technologies.

Type: New
Title: "CyberShake 3.0: Physics-Based Probabilistic Seismic Hazard Analysis"

Principal Investigator: Thomas Jordan, University of Southern California

Co-Investigators: Philip Maechling, University of Southern California
Jacobo Bielak, Carnegie Mellon University
Yefingi Cui, San Diego Supercomputer Center
Geoffrey Ely, University of Southern California
Kim Olsen, San Diego Supercomputer Center
Ricarco Taborda, Carnegie Mellon University

Scientific Discipline: Earth Sciences: Geological Sciences
INCITE Allocation: **40,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (38,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (2,000,000 processor hours)

Research Summary:

Recent destructive earthquakes including Haiti (2010), Chile (2010), New Zealand (2011), and Japan (2011) highlight the national and international need for improved seismic hazard information. What can be done to reduce the hazard from these inevitable natural events? INCITE high-performance computing resources can be used to reduce the hazards from these natural events. However, SCEC researchers need access to substantial HPC resources to apply recent computational improvements into standard seismic hazard forecasts.

SCEC will use INCITE resources to calculate an improved probabilistic seismic hazard forecast for California. The SCEC CyberShake 3.0 hazard model calculation will be based on a new USGS Unified California Earthquake Rupture Forecast 3.0 (UCERF3.0) scheduled for release by the USGS in June 2012. It will also produce a seismic hazard model for California that is directly comparable to the official USGS seismic hazard model and will show the seismic hazard community how HPC resources can improve official, broad-impact, USGS-regulated seismic hazard forecast data products. In the United States, the USGS has official regulatory authority to produce seismic hazard estimates. Official USGS seismic hazard estimates are used as inputs into state and national building code processes, thereby affecting billions of dollars in construction costs each year. Scientific improvements to seismic hazard forecasts must be accepted and adopted by the USGS before such improvements can have broad impact. SCEC, as a USGS- and NSF-funded research center, is in a unique position to pioneer, and accelerate, the application of HPC computational techniques into official, broad impact, seismic hazard forecast models.

Type: New
Title: "Direct Simulation of Fully Resolved Vaporizing Droplets in a Turbulent Flow"

Principal Investigator: Said Elghobashi, University of California-Irvine

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **20,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (20,000,000 processor hours)

Research Summary:
This project will enhance the understanding of liquid droplet vaporization and mixing processes in a turbulent flow. All liquid fuel combustion devices, mobile or stationary, use atomizers to produce sprays of fine droplets. The fuel droplets must first vaporize before their vapor mixes with the surrounding air. Understanding the physical details of the vaporization and mixing processes in a turbulent flow is an essential prerequisite to understanding the chemical reaction process and the eventual control/optimization of the energy conversion process.

This numerical study employs direct numerical simulations (DNS) to examine the two-way interactions between freely moving vaporizing droplets and isotropic turbulence. The droplets will be fully resolved in 3-D space and time, i.e., not treated as point particles, and all the scales of the turbulent motion are resolved down to the smallest relevant length- and time-scales (the Kolmogorov scales). The emphasis will be on the two-way exchange of mass, momentum, and energy between the vaporizing droplets and surrounding turbulent gas. The turbulence will be assumed isotropic as a first step before considering turbulent shear flows in future studies.

The researcher has fine-tuned his parallelized code on Intrepid, the IBM Blue Gene/P system, to make it efficiently scalable for up to 65,536 processors. The INCITE allocation on the Blue Gene/P will enable the performance of the large simulations with higher Reynolds numbers and larger numbers of vaporizing droplets. The study will be the first that fully resolves the flow inside and outside a large number of freely moving vaporizing droplets in a turbulent flow. The detailed results of the DNS, with two-way coupling between the droplets and turbulence, can be used to develop and verify the mathematical models for the subgrid scales of large-eddy simulations (LES), as well as Reynolds-averaged models. It should be emphasized that the detailed DNS data that will be obtained from the proposed research is not available to date in any published experimental or numerical study.

Type: New
Title: "Electromagnetic Effects on Gyrokinetic Simulations of Plasma Microturbulence"

Principal Investigator: Eric Wang, Lawrence Livermore National Laboratory
Co-Investigators: Jeff Candy, General Atomics
William Dorland, University of Maryland
Darin Ernst, Massachusetts Institute of Technology
Walter Guptenfelder, Princeton Plasma Physics Laboratory
William Nevins, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
The project uses two advanced plasma microturbulence codes, GYRO and GS2, for nonlinear, electromagnetic simulations of tokamak plasma microturbulence. The work aims to quantify the effects of magnetic stochasticity in realistic simulations of experiments on the three major U.S. tokamak facilities. The simulations support the SciDAC Center for the Study of Plasma Microturbulence and the Department of Energy 2012 Joint Research Target on understanding electron transport.

The project has three foci. First, an experiment in which ion temperature gradient driven turbulence dominates is based on a DIII-D tokamak shot showing beta values near the ideal ballooning limit. Work explores nonlinear pumping of electromagnetic modes capable of destroying magnetic surfaces at microscale. This work aims to develop a simulation benchmark about a realizable experiment. The second effort focuses on NSTX, where at high beta values the particle and heat transport increases with collisions. These simulations, which build on first-of-a-kind nonlinear gyrokinetic simulations of microtearing done under a previous INCITE award, allow comparison of simulated and experimental transport and turbulence. Third, we seek evidence of magnetic stochasticity by conducting an experiment in Alcator C-Mod and simulating the results. We will quantitatively compare realistic gyrokinetic simulations of magnetic stochasticity.

We search for finite-beta enhancement of the nonlinear critical density gradient for turbulence, implement strong finite ion gyroradius collisional damping terms in microtearing turbulence, and test a proposed mechanism for observed transport runaway well below magnetohydrodynamic stability limit. All projects directly impact the US fusion program goal of developing a predictive understanding of plasma transport.

Type: Renewal
Title: "Electronic Structure Calculations of Nano Solar Cells"

Principal Investigator: Lin-Wang Wang, Lawrence Berkeley National Laboratory

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: **10,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (10,000,000 processor hours)

Research Summary:
Currently, nano solar cells made of inorganic systems suffer from low efficiency, in the range of 1–3 percent. In order for the nano solar cells to have an impact in the energy market, we need their efficiencies to be above 10 percent.

The goal is to understand the mechanisms of the critical steps inside a nano solar cell. These include: the photon absorption, exciton generation, exciton dissociation, exciton and carrier decays and recombinations, carrier transport, and carrier collection. In a thin film solar cell, if the carrier diffusion constant, the impurity trapping rate, and the exciton generation rates are known, the photovoltaic process and its efficiency can be simulated by Poisson drift-diffusion equation. Some of the critical aspects of the system are still not well understood. All these are large scale simulations, which can only be carried out using INCITE allocations on the leadership facilities. Some of our codes scale to the full leadership computers.

Type: New
Title: "Enabling Green Energy and Propulsion Systems via Direct Noise Computation"

Principal Investigator: Umesh Paliath, GE Global Research
Co-Investigators: Giridhar Jothiprasad, GE Global Research
Anupam Sharma, GE Global Research

Scientific Discipline: Engineering: Energy Efficiency

INCITE Allocation: **45,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (45,000,000 processor hours)

Research Summary:
Advanced "green" energy and propulsion systems that deliver improved energy efficiency and yields from renewable sources have driven the development of accurate, high-fidelity simulation capabilities at GE Global Research. The inability of current computational fluid dynamics methods to accurately and consistently characterize turbulent mixing processes in shear flows and boundary layer flows has slowed the drive to higher efficiencies and lower emissions. A simulation methodology that captures such phenomena accurately can create a design capability with the potential to break through several barrier technologies.

GE's recent INCITE work on Large-Eddy Simulations (LES) leveraged the petascale computing enabled to break barriers relating to the aero-acoustics of wind turbine airfoils and aircraft engine jets. GE accelerated its industrial impact by pushing application/validation to realistic conditions and scale, addressing challenges, and extending capability to handle complex system interactions. Through scalability improvements at the ALCF, their past INCITE work demonstrated how this first-principles-based LES capability transforms product development.

Going forward, the researchers will demonstrate the use of scalable LES as an aero-acoustics diagnostic and design tool. Driven by recent advances in jet-engine technologies, they also plan to initiate fundamental work in fan broadband noise. The attention will shift to a harder, more subtle phenomenon from the turbulent sources generated in boundary layers and shear flows to the evolution of turbulent wakes and its interaction with stationary or moving aerodynamic surfaces downstream. For wind turbines, researchers will demonstrate accurate characterization of the complex scaling and variation of turbulent "self" noise sources to create a high-quality/fidelity database, that can be leveraged to improve lower-order noise source modeling. They also plan to push the envelope in scale to attempt 3-D tip flows. For jets, the focus will be on: (a) capturing the fundamental drivers of the next challenges in full-scale realism coming from forward-flight effects, as well as the interactions between the engine and the airframe, and (b) demonstrating the ability of LES to guide active noise control technologies beyond passive features. They expect to improve the prediction and design capabilities for next-generation aircraft engines and wind turbines.

Type: New
Title: "Energetic Aspects of CO_2 Absorption by Ionic Liquids From Quantum Monte Carlo"

Principal Investigator: William A. Lester, Jr., University of California-Berkeley

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **4,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (4,000,000 processor hours)

Research Summary:
This quantum Monte Carlo (QMC) investigation of interaction energies between imidazolium-based ionic liquids (ILs) and CO_2 will lead to a comprehensive model of CO_2 absorption by ILs. The project is a crucial component of creating a solid framework of computational results that can be used by researchers to develop comprehensive models for CO_2 capture.

ILs hold great promise for CO_2 capture technologies — in the coal and natural gas power industries, for example — because they are less hazardous than organic solvents and have favorable properties for energy-efficient carbon capture.

The QMC method ensures highly accurate treatment of weak interactions, which will help resolve discrepancies in existing theoretical results that have hindered comprehensive modeling of CO_2 capture technologies. Obtaining accurate knowledge of interaction energies is critical to realizing IL's potential for industrial-scale technologies for CO_2 capture.

Type: New
Title: Fault-Oblivious Exascale Computing Environment

Principal Investigator: Ronald Minnich, Sandia National Laboratories
Co-Investigators: Jonathan Appavoo, Boston University
Maya Gokhale, Lawrence Livermore National Laboratory
Sriram Krishnamoorthy, Pacific Northwest National Laboratory
Ponnusamy Sadayappan, Ohio State University
Eric Van Hensbergen, IBM Research

Scientific Discipline: Computer Science

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
Two areas of concern that have emerged from several DOE meetings on exascale systems (machines with 100 million cores) are runtime systems which can function at that scale, and fault management. The Fault Oblivious Exascale (FOX) project aims to build a software stack that combines the management of these two issues; a work-queue based runtime which is designed to naturally accommodate failure as just another event in which a computational component failed to complete.

The team is exploring fault isolation and recovery across the entire stack from the operating system, through the runtime, up into the application. The core of this approach is based upon a fault-tolerant distributed data store, and a task management system built on top of that. The approach will provide both file system interfaces to these systems services, as well as more tightly coupled runtime interfaces to support a wide range of programming models. As there are no exascale systems, INCITE time on a petascale system will be used to test the FOX environment, specifically:

- New quantum chemistry kernel implementations using a work queue mode, developed by PNNL, SNL and OSU.
- A petascale implementation of a distributed data store based on Kyoto Cabinet, being ported to HPC platforms by LLNL and SNL.
- SESA, a new HPC OS for petascale systems, developed by BU, IBM and U. Karlsruhe.
- An asynchronous graph traversal application based on a distributed work-queue model, developed at LLNL.

The result of this work will be new applications environments for DOE use, and results from software and library development that the vendor can use to guide development of future exascale systems.

Type: Renewal
Title: "High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry"

Principal Investigator:	William George, National Institute of Standards and Technology (NIST)
Co-Investigators:	Edward Garboczi, NIST Pascal Hebraud, CNRS/ESPCI – France Nicos Martys, NIST Marc Olano, NIST Judith Terrill, NIST

Scientific Discipline:	Rheology
INCITE Allocation:	**22,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/P (22,000,000 processor hours)

Research Summary:
Flow properties of large-particle suspensions, such as concrete, cannot now be measured accurately in industrial settings. Flow simulations with many thousands of particles with a wide range of sizes and shapes in a non-Newtonian fluid matrix will enable the design of rheometers that will revolutionize the use of these instruments. The project's previous three-year INCITE award, granted in 2008, gave researchers the computing power to perfect their algorithms and to test parameters such as system size and the width of the size distribution of the suspended particles in a large-scale parallel approach. The researchers now seek to apply this capability to very large-scale parallel simulations needed to solve the problem of quantitatively extracting fundamental rheological parameters such as stress and strain rate from measured quantities such as torque and angular velocity in non-analytical rheometer and mixing geometries. Analysis and visualization of the simulated flow will enable the researchers to develop a fundamental framework to understand important physical mechanisms that control the flow of such complex fluid systems. Results from this study will advance the science of dense suspensions and enable the measurement science needed for rheometer design for these systems. This will solve a critical outstanding problem in the cement and concrete industry, and will also have an enormous influence on the wide array of industries that use vane rheometers and mixers, from food processing to water treatment, to coatings, and to pharmaceuticals.

Type: Renewal
Title: "High-Fidelity Simulations for Advanced Engine Combustion Research"

Principal Investigator: Joseph Oefelein, Sandia National Laboratories
Co-Investigators: Jacqueline Chen, Sandia National Laboratories
Ramanan Sankaran, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **65,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (65,000,000 processor hours)

Research Summary:
Transportation by automobiles and trucks in the United States accounts for two-thirds of our oil use and one-fourth of our greenhouse gas emissions. Thus, the interdependent advancement of both fuel and engine technologies is a key component of the strategy to dramatically reduce both oil consumption and greenhouse gases.

The calculations proposed here aim to contribute to this goal through development of advanced predictive capabilties for turbulent combustion processes in internal-combustion (IC) engines. We will apply an optimal combination of large eddy simulations, direct numerical simulations, and molecular dynamics simulations to provide new insights with respect to key phenomenological processes and further refinement and validation of key sub-models. While the focus of the current effort is on IC-engines, it should be noted that the challenges and approach described here apply to any propulsion and power device. The collaborative effort is supported by a portfolio of five DOE funded projects with collaborative links and strong coupling to a companion set of experiments. These projects directly address targeted research areas identified as part of a BES sponsored workshop entitled Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels. The major goals of the effort are 1) to provide new insights into the dynamics of turbulent combustion processes in IC-engines, and 2) maximize the collective benefits of these insights through synergistic collaborations between the sub-groups of researchers involved.

Type: Renewal
Title: "How High Redshift Galaxies Reionized the Universe"

Principal Investigator: Michael Norman, University of California-San Diego
Co-Investigators: Robert Harkness, San Diego Supercomputer Center
Daniel Reynolds, Southern Methodist University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **32,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (32,000,000 processor hours)

Research Summary:
Our objective is to critically test whether the population of high redshift galaxies discovered by the *Hubble Space Telescope* are capable of reionizing the universe consistent with observational constraints using self-consistent cosmological radiation hydrodynamical simulations.

We plan to critically test the dwarf galaxy reionizer hypothesis with self-consistent cosmological radiation hydrodynamical simulations of unprecedented scale. Our simulations differ from what has been done previously in two important respects: 1) rather than treat the ionizing flux of a dwarf galaxy as a free parameter, we will calibrate our model using the latest *Hubble Space Telescope* observations. Second, our simulations will self-consistently evolve the dark matter, baryonic matter, ionizing radiation, ionization balance, and gas photoheating on the same high resolution grid within large cosmological volumes. This is a petascale application because of the large range of relevant scales (about 10,000 in 3D) that must be simulated simultaneously and self-consistently, and the compute-intensive nature of radiation hydrodynamic simulations. The simulations must cover a large enough range of scales to include the relative contribution of galaxies of different mass and luminosity to the reionization process. These will be the first fully self-consistent simulations of reionization at high enough resolution and in large enough volumes and to engage multiple observations to critically test the dwarf galaxy reionizer hypothesis.

Type: Renewal

Title: "Investigation of Multi-Scale Transport Physics of Fusion Experiments Using Global Gyrokinetic Turbulence Simulations"

Principal Investigator: Weixing Wang, Princeton Plasma Physics Laboratory

Co-Investigators: Mark Adams, Columbia University
Stephane Ethier, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Wei-li Lee, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **19,000,000 processor hours**

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XK6 (19,000,000 processor hours)

Research Summary:

The development of magnetic fusion as a secure and reliable energy source that is environmentally and economically sustainable is a formidable scientific and technological challenge in the 21st century. Understanding heat and particle losses caused by plasma turbulence in magnetic fusion devices is especially important for the next generation of burning plasma experiments such as international ITER reactor because the size and cost of a fusion reactor are expected to be largely determined by the balance between these energy losses and the self-heating rates of the actual fusion reaction. Accordingly, the control and possible suppression of turbulence caused by plasma microinstabilities is a major area of ongoing research of which advanced numerical simulations is a prominent component.

This petascale simulation project will investigate the physics of turbulence-driven momentum, energy, and particle transport, and their relationship to tokamak fusion experiments. The focus will be on the nonlinear physics occurring on multispatial and multitemporal scales involving both ion and electron dynamics. Our numerical studies will emphasize i) the physics validation of our simulation model against results from the three major fusion experiments in the United States, namely NSTX, DIII-D and C-MOD, and ii) the application of predictive capability in these simulation tools for assessing critical plasma confinement issues associated with ITER. Reliable predictions of the confinement properties in modern laboratory fusion experiments will require global kinetic simulations with multi-scale resolution—a true grand challenge that will require petascale computing capabilities.

Type: Renewal
Title: "Large-Eddy Simulation of Two-Phase Flow Combustion in Gas Turbines"

Principal Investigator: Thierry Poinsot, CERFACS
Co-Investigators: Gabriel Staffelbach, CERFACS

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
Using the capability of the Blue Gene/P supercomputer, CERFACS has been performing top-of-the-line, quality simulations on highly complex cases to numerically model a real combustor. The project focuses on Large Eddy Simulation (LES) of these engines with the inclusion of the liquid phase phenomena. With this in mind, CERFACS has performed simulations and validation of two-phase flow experiments.

In parallel, CERFACS has performed the largest unstructured LES to date on a full commercial combustion chamber (330 million elements). This simulation contributes to the validation of the LES approach when dealing with combustion instabilities, where the high unsteadiness of the flow makes the impact of the uncertainty behind the LES combustion model a highly critical point that needs to be addressed.

Using LES, the researchers can predict combustion instability in an annular combustion chamber. Their data suggests that the liquid phase is less sensitive to the increased resolution but confirms that LES models applied to combustion of gaseous or liquid fuels degenerate towards fully resolved, direct numerical simulation when they increase the mesh resolution.

Following these studies, they have focused on the impact of fuel properties changes on the overall behavior of the turbine. Using the LES that revealed fully developed azimuthal instability, they simulated the use of a faster fuel under the same conditions. Preliminary results show that not only is LES capable of accounting for this change but such a modification can yield important optimization results. In this case, by changing the fuel they were able to stabilize the system where the pressure fluctuation amplitude drops dramatically just after the change while conserving the overall topology of the flame and the flow. These results give potential hints to the gas turbine designer to avoid combustion instability. Their analysis also suggests that decreasing the response time of the burner (a typical parameter of turbines) would stabilize this combustor design. The findings show the potential of using LES for the numerical study of combustion in alternative fuels. The work is still in progress, with further analysis under way.

Type: New
Title: "Large-Eddy Simulations of Contrail-to-Cirrus Transition"

Principal Investigator: Roberto Paoli, CERFACS
Co-Investigators: Juan Escobar, Laboratoire d'Aérologie
Odile Thouron, CERFACS

Scientific Discipline: Earth Science: Environmental Sciences

INCITE Allocation: **20,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (20,000,000 processor hours)

Research Summary:
Aircraft emissions can affect the chemical composition of the atmosphere and modify or create additional ice clouds in the form of contrails. When contrails spread to form cirrus clouds, they can persist for hours and extend over areas of several square kilometers. These "contrail cirrus," which artificially increase Earth's cloudiness and become almost indistinguishable from natural cirrus, are among the most uncertain contributors to the Earth's radiative forcing. With this project, researchers will use large-eddy simulations to fully understand the physics of the formation of contrail cirrus, and provide a valuable contribution to the development of parameterizations of aircraft-induced cirrus in next-generation global and climate models.

One of the critical aspects of this problem is represented by the transition between contrail and cirrus that occur when the effects of the atmospheric perturbations become predominant, compared to the dynamics of the aircraft wake where ice particles are initially trapped. From a modeling point of view, this is a challenging task because of the multiple complex physical phenomena involved including atmospheric turbulence, radiative transfer, and microphysics. This project will also require large computational domains to accommodate the spreading of the contrail and high resolution to correctly capture the mixing with the ambient air. By understanding and characterizing the physical mechanisms that control the formation of contrail cirrus, this work will lead to more complete and effective climate models in the future.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul B. Mackenzie, Fermi National Accelerator Laboratory
Co-Investigators: Richard C. Brower, Boston University
Norman H. Christ, Columbia University
Frithjof Karsch, Brookhaven National Laboratory
Julius Kuti, University of California—San Diego
John W. Negele, Massachusetts Institute of Technology
David G. Richards, Jefferson Laboratory
Stephen R. Sharpe, University of Washington
Robert Sugar, University of California—Santa Barbara

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **96,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (50,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (46,000,000 processor hours)

Research Summary:
In 2012 researchers intend to dramatically advance research in lattice quantum chromodynamics and other strongly coupled field theories of importance to the study of high energy and nuclear physics. This project will deepen scientists' understanding of the interactions of quarks and gluons, the basic components of 99% of the visible matter in the universe, and will play an important role in ongoing efforts to develop a unified theory of the four fundamental forces of nature. These fundamental questions in high energy and nuclear physics are directly related to major experimental programs and milestones set out by the Department of Energy's Office of Science.

To date, this project has created several ensembles of gauge configurations that have been analyzed for a rich set of experimental applications. It has already produced the most accurate determinations of the strong coupling constant and the light quark masses ever achieved. It has produced the most accurate determinations of several elements of the CKM matrix in existence. It has produced detailed spectra of the excited mesons and baryons that will be studied in Jefferson Lab experiments. It is producing new ensembles of configurations that will be of even greater importance to the experimental programs of high energy and nuclear physics.

Type: New
Title: "Magnetic Reconnection in High-Energy-Density Laser-Produced Plasmas"

Principal Investigator: Amitava Bhattacharjee, University of New Hampshire
Co-Investigators: Naoki Bessho, University of New Hampshire
William Fox, University of New Hampshire
Kai Germaschewski, University of New Hampshire
Yi-Min Huang, University of New Hampshire

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
Magnetic reconnection—the process by which the magnetic topology in plasmas is rearranged—is ubiquitous in fusion, space and astrophysical plasmas. It is widely believed to play a central role in phenomena as diverse as sawtooth crashes in fusion plasmas, magnetospheric substorms, and solar flares, which are among some of the most challenging problems in plasma physics.

This project focuses on magnetic reconnection as observed in high-energy-density (HED), laser-produced plasmas in the presence of extremely high magnetic fields. The computations are central to the DOE Experimental Program to Stimulate Competitive Research's Center for Integrated Computation and Analysis of Reconnection and Turbulence. It is a main premise of the center that fundamental aspects of magnetic reconnection and turbulence in fusion devices, smaller-scale laboratory experiments, and space and astrophysical plasmas can be viewed from a common perspective, and that progress in understanding in any of these interconnected fields is likely to lead to progress in others.

Recent experiments on magnetic reconnection in HED laser-produced plasmas open up a new experimental regime, potentially of interest for plasma astrophysics as well as inertial fusion energy applications. This project seeks to improve our understanding of these experiments and this general regime of reconnection in large systems at the intersection of kinetic, collisional, and two-fluid effects, through a detailed comparison of computation (including both kinetic and fluid codes) with experiment, with the goal of bringing the two into quantitative agreement.

Type: Renewal
Title: "Magnetic Structure and Thermodynamics of Low Dimensional Magnetic Structures"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Don Nicholson, Oak Ridge National Laboratory
Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **46,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (46,000,000 processor hours)

Research Summary:
This project will explore the energy landscape of low dimensional magnetic structures (LDMS) that are free standing, adsorbed on surfaces, and embedded in the bulk. Within bulk magnetic materials, all defects are LDMS, having spin arrangements that differ from their surroundings. The properties of LDMSs lead to novel responses to electric, magnetic, and stress fields that may result in important logic, memory, optical, and structural applications. In many materials, typically steels, magnetic defects are important to strength and fracture toughness. The goal of this work on LDMS is to understand their low-temperature magnetic structure and their thermodynamic fluctuations at higher temperature. This understanding can lead to advances in energy and information applications and to stronger, lighter materials for increased energy efficiency. The work will advance the overall objectives of the Office of Science and will contribute to and benefit from modeling and experimental work in the Energy Frontier Center for Defect Physics in Structural Materials.

Type: New
Title: "Mixing in Incompressible and Compressible Turbulence"

Principal Investigator: Pui-kuen Yeung, Georgia Institute of Technology
Co-Investigators: Diego Donzis, Texas A&M University
Toshiyuki Gotoh, Nagoya Institute of Technology
Dmitry Pekurovsky, San Diego Supercomputer Center
Katepalli Sreenivansan, New York University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **28,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (28,000,000 processor hours)

Research Summary:
Turbulent mixing often plays a rate-limiting role in technological applications such as heat and mass transfer in industrial processes, pollutant dispersion, and the mixing of fuel with air in aircraft engines.

For mixing in incompressible turbulence the main target in this proposal is the regime of a very low Schmidt number, corresponding to high molecular diffusivity which is typical in liquid-metal applications, where laboratory data are not readily available. Recent simulations at low Reynolds numbers have shown that usual spectral cascade paradigms do not apply, leading to many unconventional behaviors at small scales, which in turn will have an impact on modeling. For compressible turbulence, the velocity field itself is much less understood and prior simulations (which are more expensive on a per-grid-point basis) in the literature have been limited. An issue of special interest is the role of eddy shocklets representing strong local compression, which may tend to amplify scalar gradients at small scales.

This project emphasizes that in both problems above the aim is at simulations of world-class resolution, designed to probe deeply long-unresolved fundamental and practically important questions in turbulence theory. In conjunction with other projects in the U.S. and Japan, this project is also actively exploring further performance improvements in our already highly scalable codes.

Type: Renewal
Title: "Multiscale Blood Flow Simulations"

Principal Investigator: George Karniadakis, Brown University
Co-Investigators: Leopold Grinberg, Brown University
Vitali Morozov, Argonne National Laboratory
Michael Papka, Argonne National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **73,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (50,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (23,000,000 processor hours)

Research Summary:
Cerebral aneurysms occur in up to 5% of the general population, leading to strokes in over 40,000 Americans each year. Sickle cell anemia, a chronic inflammatory disease, is the most common genetic disease among African Americans, with an 8% incidence of the trait in this population; 50,000 individuals battle sickle cell anemia in the United States each year. Cerebral malaria is a related disease of the red blood cells, with mortality at up to 20%, even with treatment. More than 1.5 million deaths are reported annually, chiefly in children.

No quantitative tools exist to predict aneurysms or the progression of conditions like sickle cell anemia or cerebral malaria. Researchers are using the power of supercomputers to create realistic simulations of these brain pathologies, quantifying their biophysical characteristics for the first time. Through physiologically correct multiscale simulations of the human brain vasculature, scientists are able to model blood flow in the human brain vasculature, the first of its kind, consisting of hundreds of large 3-D arteries (Macrovascular Network, MaN), 10M arterioles (Mesovascular Network, MeN) and 1B capillaries (Microvascular Network, MiN).

To date, the team has achieved the following:

- Simulated the initial stages of clot formation using a coupled continuum-dissipative particle dynamics solver.
- Simulated blood flow at various levels of hematocrit and healthy and diseased red blood cells. Studied the mechanical properties of glycocalyx.
- Studied microcirculation in bifurcating arteries.
- Studied the conditions for the eventual rupture of an aneurysm.

Type: New
Title: "Multiscale Modeling of Energy Storage Materials"

Principal Investigator:	Gregory A. Voth, University of Chicago and Argonne National Laboratory
Scientific Discipline:	Materials Science: Condensed Matter and Materials
INCITE Allocation:	**25,000,000 processor hours**
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/P (25,000,000 hours)

Research Summary:
The leadership-class computing resources provided by the INCITE program will be used for the multiscale modeling of charge transport processes in materials relevant to fuel cell and battery technologies. Computational modeling of such systems seeks to address the poorly understood ion conduction mechanisms in fuel cell membranes and electrode-electrolyte interfaces in batteries. Both systems carry unique challenges that will be addressed by developing methods that are both systematic across several length scales and predictive for materials design. Atomistic-scale simulations of materials will be connected via a multiscale bridge to coarse-grained models to understand the transport of water and ions in polymer electrolyte membranes with irregular morphology and Li-ion batteries under applied potentials. This approach can significantly impact the chemistry and materials science communities by providing multiscale methods, as well as tools for the design of next-generation fuel cells and batteries.

Ion conduction in fuel cell membranes will focus on the proton transport properties of polymer electrolyte membranes, such as DuPont's Nafion. Due to the amorphous nature of these materials and the complex H-bond rearrangement that coincides with the transport of protons and hydroxide ions, multiple time and length scales are necessary to properly understand the diffusion properties through these porous media. The results of large-scale, all-atom simulations will be used to systematically and rigorously develop coarse-grained models for use in larger-scaled simulations to investigate domain formation and its coupling to diffusion processes through these membrane materials. Secondly, the molecular mechanism for charge transport at electrode interfaces will be investigated during the charging/discharging process in Li-ion batteries. The methodology will address the ion conductivity at the electrode interface with the inclusion of solvation dynamics, applied electric fields, and heterogeneous environment of the solid electrolyte interphase. This work meets the challenges of modeling energy storage materials at the mesoscale by rigorously connecting atomistic detail to macroscopic transport properties through accessing the large length and time scales in complex condensed phase environments that affect ion transport.

Type: Renewal
Title: "Nuclear structure and nuclear reactions"

Principal Investigator:	James Vary, Iowa State University
Co-Investigators:	Joseph Carlson, Los Alamos National Laboratory Pieter Maris, Iowa State University Hai Ah Nam, Oak Ridge National Laboratory Petr Navratil, Lawrence Livermore National Laboratory Witold Nazarewicz, University of Tennessee Steven Pieper, Argonne National Laboratory Nicolas Schunck, Oak Ridge National Laboratory

Scientific Discipline:	Physics: Nuclear Physics
INCITE Allocation:	**55,000,000 processor hours**
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK6 (37,000,000 processor hours)
Site:	Argonne National Laboratory
Machine (Allocation):	IBM Blue Gene/P (18,000,000 processor hours)

Research Summary:
Developing a comprehensive description of all nuclei (stable and unstable) and their reactions requires investigations of rare and exotic isotopes with unusual proton-to-neutron ratios that are difficult to produce and study experimentally because of their short lifetimes. We perform state-of-the-art simulations to provide needed predictions where direct experiment is not possible or is subject to large uncertainties.

Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs. Such calculations are relevant to many applications in nuclear energy, nuclear security and nuclear astrophysics, where rare nuclei lie at the heart of nucleosynthesis and energy generation in stars.

Type: New
Title: "Optimization of Complex Energy System Under Uncertainty"

Principal Investigator: Mihai Anitescu, Argonne National Laboratory
Co-Investigators: Cosmin Petra, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Energy Grid

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
The U.S. electrical power system is at a crossroads between its mission to deliver cheap and safe electrical energy, a strategic aim to increase the penetration of renewable energy, an increased reliance on smart grid technology, and the critical need to maintain and increase the reliability of the grid. Additionally, the operation and planning of the grid with these requirements involves an unprecedented amount of uncertainty in supply and demand brought on by the high variability of wind, solar, and other renewable power sources.

This project will develop advanced optimization methods for the power grid under uncertainty, with the aim of ensuring efficient, reliable, cost-effective, and sustainable electrical energy operations. Specifically, researchers will investigate the modeling of stochastic power grid optimization on massively parallel supercomputers. In this particular case, stochastic programming is a leading formulation that uses optimization under uncertainty to balance the variability in the wind supply with its benefits in the context of operational reliability.

The project's main technical challenges are that the tasks involved are highly computationally intensive, they must run under strict time constraints, and they must run at a high frequency to properly manage the large real-time fluctuations of supply and demand. This project will solve optimization problems of unprecedented size (tens of billions variables and constraints), which will also help to advance the field of mathematical optimization.

Type: Renewal
Title: "Performance Evaluation and Analysis Consortium End Station"

Principal Investigator: Patrick Worley, Oak Ridge National Laboratory
Co-Investigators: David H. Bailey, Lawrence Berkeley National Laboratory
Jack J. Dongarra, University of Tennessee
William D. Gropp, University of Illinois at Urbana-Champaign
Jeffrey K. Hollingsworth, University of Maryland
Robert F. Lucas, University of Southern California
Allen D. Malony, University of Oregon
John Mellor-Crummey, Rice University
Barton P. Miller, University of Wisconsin at Madison
Leonid Oliker, Lawrence Berkeley National Laboratory
Allan Snavely, University of California at San Diego
Jeffrey S. Vetter, Oak Ridge National Laboratory
Katherine A. Yelick, University of California at Berkeley
Bronis R. de Supinski, Lawrence Livermore National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation: **28,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (18,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
To maximize the utility of Department of Energy leadership class systems, we must understand how to use each system most efficiently. The performance community (performance tool developers, performance middleware developers, system and application performance evaluators, and performance optimization engineers) can provide the tools and studies to enable these insights, if they have adequate access to the systems.

To provide further understanding of these high-end systems, this proposal focuses on four primary goals: (1) update and extend performance evaluation of all systems using suites of both standard and custom micro, kernel, and application benchmarks; (2) continue to port performance tools and performance middleware to the leadership class systems; (3) validate the effectiveness of performance prediction technologies, modifying them as necessary to improve their utility for predicting resource requirements for production runs on the leadership-class systems; and (4) analyze and help optimize current or leadership class application codes.

Type: Renewal
Title: "Petascale Modeling of Chemical Catalysts and Interfaces"

Principal Investigator: Robert Harrison, Oak Ridge National Laboratory
Co-Investigators: Edoardo Apra, Oak Ridge National Laboratory
David Dixon, University of Alabama
Karol Kowalski, Pacific Northwest National Laboratory
William Shelton, Pacific Northwest National Laboratory
David Sherrill, Georgia Institute of Technology
Bobby Sumpter, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Catalytics

INCITE Allocation: **46,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (46,000,000 processor hours)

Research Summary:
In this proposal, we refocus our prior INCITE project on the central science theme of understanding, controlling, and ultimately designing catalytic chemical processes with special interest in surfaces that are relevant to diverse battery technologies, ultra-capacitors, fuel cells, environmental chemistries, and catalytic processes for sustainable energy production including biomass conversion. This is a grand-challenge and cross-cutting problem that, in close partnership with experiment and theory, requires sustained progress over the coming decade starting now with petascale and eventually with exascale computers. This fundamental science topic and the essential integration of experiment with the required new theory and advanced computational tools have been identified as proposed or cross-cutting research directions in multiple Basic Research Needs (BRN) reports including "BRN to Assure a Secure Energy Future, "BRN for Solid State Lighting", "BRN for Electrical Energy Storage," and "BRN Catalysis for Energy." Theoretical simulations output of this proposal are structured to deliver "a significant increase in the rate of discovery, innovation and technological change'" (from BES report "New Science for a Secure and Sustainable Energy Future") in energy storage and production. The cross-cutting simulation capabilities will, by design, have immediate impact also on biomass conversion, inorganic and organic photo-voltaics, and the heavy-element chemistries that are vital to diverse DOE missions.

Type: Renewal
Title: "Petascale Modeling of Nano-electronic Devices"

Principal Investigator: Gerhard Klimeck, Purdue University
Co-Investigators: Benjamin Haley, Purdue University
Mathieu Luisier, Purdue University
Tillman Kubis, Purdue University
Hong-Hyun Park, Purdue University
Michael Povolotskyi, Purdue University

Scientific Discipline: Materials Science: Nanoelectronics

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
With the advent of nanoscale fabrication, a new generation of nanoelectronic devices is expected to produce enormous advances not only in computing and information technologies, but also in other fields such as medicine. The new generation of device models is atomistic and needs to account for strain, surface roughness, disorder, and impurities that can affect properties and performance of nanoelectronic devices. Whereas classical physics was used to build very successful semiconductor device models in the past, nanoscale devices require a quantum mechanical description to correctly model properties of the device.

Resonant tunneling diodes, quantum dots, and nanowires are examples of new nanoscale devices that we can model with the packages we have developed. We also compute the electronic structure of nanodevices using an empirical tight-binding basis, for tens of millions of atoms. A quantum mechanical description of a device brings a significantly greater modeling and computing challenge. Our codes have been shown to scale to 32,000 cores (1 billion atoms) for the electronic structure model and 222,720 cores for the quantum transport model. This work will enable discovery of new technologies for faster switching, smaller feature size, and reduced heat generation. The creation of new switch technology will revitalize the semiconductor industry in 2015. Designers will be enabled to directly address questions of quantization and spin, tunneling, phonon interactions, and heat generation for nanoscale devices.

Type: Renewal
Title: "Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"

Principal Investigator: Warren Mori, University of California, Los Angeles
Co-Investigators: Frank Tsung, University of California, Los Angeles

Scientific Discipline: Physics: Accelerator Physics

INCITE Allocation: **19,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (19,000,000 processor hours)

Research Summary:
The long-term future of experimental high-energy physics research using accelerators depends on the successful development of novel ultra-high-gradient acceleration methods. New acceleration techniques using lasers and plasmas have already been shown to exhibit gradients and focusing forces more than 1,000 times greater than conventional technology, raising the possibility of ultra-compact accelerators for applications in science, industry, and medicine. Plasma-based accelerators have been a fast-growing field due to a combination of breakthrough experiments, parallel code developments, and a deeper understanding of the underlying physics of the nonlinear wake excitation in the so-called blowout regime. Based on this progress in experiment, theory, and simulation, linear collider concepts using wakefields have been developed and two facilities approved. One is Facilities for Accelerator Science and Experimental Test Beams (at the SLAC National Accelerator Laboratory).

This facility will provide 25 GeV electron and positron beams. The other facility is the Berkeley Lab Laser Accelerator (at Lawrence Berkeley National Laboratory). It will provide a 30-Joule/30-femtosecond laser. The goal for each facility is to experimentally test key aspects of a single cell within the collider concepts. Furthermore, there are other lasers both within the United States and in Europe and Asia that are or will be able to experimentally study laser wakefield acceleration in nonlinear regimes. While some simulations will be conducted to help design and interpret near-term experiments, the main goal of this proposal is to use these advanced simulation tools to study parameters that are in regimes that will not be accessible. We will, therefore, dramatically advance the rate of discovery and progress in plasma-based accelerator research.

Type: New
Title: "Petascale PIC Simulations of Laser-Plasma Interactions in IFE Plasmas"

Principal Investigator: Frank Tsung, University of California, Los Angeles
Co-Investigators: Warren Mori, University of California, Los Angeles

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
UCLA's plasma simulation group has a long history of expertise in particle-in-cell (PIC) simulations, leadership-class computing, data reduction and visualization, and laser and beam-plasma interactions. It may have the most complete set of PIC parallel computing tools for modeling high frequency physics in high energy density plasmas. The project applies these tools and expertise to study laser plasma interactions (LPI) on spatial and temporal scales relevant to inertial fusion energy (IFE) scenarios. LPI remains one of the biggest obstacles to IFE.

Recently, the National Ignition Facility has been delivering more than one mega-joule on target for the first time, while simultaneously other higher gain IFE schemes like shock ignition are also being pursued in other laser facilities such as OMEGA. We aim to study high frequency laser-plasma instabilities that can absorb, deflect, or reflect laser light and generate energetic electrons. Such processes can limit the laser intensity in both direct and indirect drive IFE scenarios, limiting overall gain. In conventional IFE, fast electrons can preheat the target. Two important instabilities—two-plasmon decay and stimulated Raman scattering–spur fundamental plasma physics questions on nonlinear plasma waves. These processes both depend on the local electron distribution function and can lead to electron distribution functions that are severely modified near the phase velocity of the plasma's wave and that include fast electron tails. Thus, understanding them requires multi-dimensional fully kinetic models.

Complex and highly nonlinear, the physics of these processes involves both wave-wave and wave-particle interactions, necessitating fully nonlinear and fully kinetic computer models. The goal is to have a hierarchy of kinetic, fluid, and other reduced description approaches that can model full space and time scales. One critical piece is fully explicit PIC in which Maxwell's equations are solved on a grid using currents and charge densities calculated by weighting discrete particles onto the grid. Each particle is pushed to a new position and momentum via self-consistently calculated fields. The difficulty in applying fully explicit PIC codes is that they are computer intensive, so that the spatial and temporal scales that can be modeled are limited. However, the unprecedented computing power of today's leadership class facilities make it possible to use highly optimized codes to study problems of interest to the IFE program.

Type: New
Title: "Petascale Simulations of Inhomogeneous Alfven Turbulence in the Solar Wind"

Principal Investigator: Jean C. Perez, University of New Hampshire
Co-Investigators: Benjamin Chandran, University of New Hampshire

Scientific Discipline: Physics: Solar/Space Physics

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
This project's large-scale numerical simulations of Alfvén wave (AW) turbulence in the outermost atmosphere of the sun will lead to new insights into the basic properties of inhomogeneous AW turbulence and make a major contribution to scientists' understanding of coronal heating and the origin of the solar wind.

The project will carry out the first direct numerical simulations of AW turbulence in the extended solar atmosphere that account for inhomogeneities in the density (ρ), flow speed (U), and background magnetic field (B_0) within a narrow magnetic flux tube extending from roughly one solar radius to eleven solar radii. Numerical simulations will be compared with remote observations.

NASA's Solar Probe Plus mission in 2018 to uncover the origin of the solar wind will send a spacecraft inside the solar atmospheric region that this project will simulate numerically. The simulations of this project will enable detailed comparisons with future spacecraft measurements, contributing significantly to the science return of this pioneering mission.

Type: Renewal
Title: Petascale Simulations of Stress Corrosion Cracking

Principal Investigator: Priya Vashishta, University of Southern California
Co-Investigators: Aiichiro Nakano, University of Southern California

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **45,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (45,000,000 processor hours)

Research Summary:
The performance and lifetime of materials widely used in energy and nuclear technologies are often severely limited by corrosion under stress loads. Particularly important for the DOE are environmental degradations of nickel-based alloys in advanced nuclear reactors and in glass containers of nuclear waste.

This team performs petascale reactive molecular dynamics (MD) and quantum mechanical (QM) simulations to investigate fundamental mechanisms of stress corrosion cracking (SCC) and nanoindentation of silica glass in the presence of water as well as impurity segregation-induced embrittlement of nickel-aluminum alloys.

In order to prevent SCC and to predict the lifetime beyond which SCC may cause failure, the petascale hierarchical simulation approach is used to discover:

- The role of water in nanoindentation damage of silica glass;
- Fundamental mechanisms of SCC in silica glass in the presence of water; and
- Atomistic mechanisms of impurity (sulfur and boron)-segregation induced embrittlement in nickel-aluminum alloys.

In the first year of the project, the team performed a billion-atom reactive MD simulation to study silica-water chemistry at a nanoindent on a silica surface generated by the collapse of a cavitation nanobubble in water, thus revealing the role of water in nanoindentation damage. In 2012, the team will carry over this knowledge to large-scale QM and reactive MD simulations to identify fundamental mechanisms of SCC in silica glass in the presence of water. The simulations of silica glass in the presence of water will be based on interatomic potentials that incorporate reactive processes involving bond breaking and bond formation as well as dynamic atomic charges that change with changes in the local atomic configurations. This will determine changes in the structure and surface energy of silica glass in the presence of water. Accelerated MD simulations will be performed to determine the dependence of the cracking initiation load in water.

Type: New
Title: "Petascale Simulations of Type Ia Supernovae"

Principal Investigator: Stan Woosley, University of California-Santa Cruz
Co-Investigators: John Bell, Lawrence Berkeley National Laboratory
Mike Zingale, SUNY-Stony Brook
Dan Kasen, University of California, Berkeley

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **46,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (46,000,000 processor hours)

Research Summary:
Type Ia supernovae (SN Ia) are the largest thermonuclear explosions in the modern universe. Because of their brilliance and nearly constant luminosity at peak, they are also a "standard candle" favored by cosmologists to measure the rate of cosmic expansion. Yet, after 50 years of study, no one really understands how SN Ia work. The model that agrees best with observations is an exploding white dwarf star in which carbon and oxygen fuse in a runaway process that makes chiefly elements in the iron group. Most of the iron in the universe has been created this way, but just how the white dwarf ignites and burns is a difficult problem in turbulent combustion, comparable in complexity to a first principles modeling of what goes on in an automobile engine. The burning ignites in a chaotic convective flow, which makes the location hard to determine, and the ashes that the burning produces are buoyant. Their rise leads to instabilities and turbulence that modify the burning rate in a way that is difficult to calculate. Only recently have the necessary codes been written, and only with petascale machines is the problem numerically tractable.

Here, we propose an "end to end", first principles, simulation of a SN Ia using three codes that have been developed for this purpose with support from the DOE SciDAC Program. Each code has been demonstrated to scale, for this particular problem, on over 100,000 CPU on Jaguar. MAESTRO, our low-Mach-number AMR code, is unique in its ability to finely resolve the convective flow that precedes ignition. The nuclear burning is turbulent and must be resolved, initially at least, on sub-km scales in a star 2000 km in radius. The integral scale of the turbulence is ~10 km and this must be resolved as the supernova expands to about 10,000 km. Finally, the 3D explosion will be post-processed using our Monte Carlo code, SEDONA, to obtain the light curve and spectra.

Type: Renewal
Title: "Potential Energy Surfaces for Simulating Complex Chemical Processes"

Principal Investigators: Donald G. Truhlar, University of Minnesota
Osanna Tishchenko, University of Minnesota
Co-Investigators: Jingjing Zheng, University of Minnesota

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **15,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)

Research Summary:
Large-scale electronic structure theory provides potential energy surfaces and force fields for simulating complex chemical processes important for technology and biological chemistry. Addressing the challenge of obtaining accurate energies and stationary points for systems whose electronic structure has high multi-reference character, the researchers use multi-reference perturbation theory (MRMP2) and multi-configuration quasi-degenerate perturbation theory (MCQDPT). The team applies MRMP2 and MCQDPT to study three classes of reactive systems in the gas phase and materials: (1) charge transfer coupled to magnetic spin state change in metallofullerenes and metal-doped carbon nanotubes, (2) reactions of phenolic antioxidants with free radicals, and (3) radical–radical and radical–molecule association reactions.

The first class of problems is important for achieving a fundamental understanding of charge transfer and polarity in the context of molecular electronics and spintronics. The second class of problems is important for developing clean and efficient fuels and understanding atmospheric chemistry. The project also includes two exploratory subprojects: (1) density functional theory for catalytic reactions at gas–solid and gas–nanoparticle–solid interfaces and for charge transfer at material interfaces, and (2) non-collinear density functional theory calculations for understanding catalysis, materials, and nanoclusters with interesting magnetic properties and the general bonding process.

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

Type: New
Title: "Precision Many-Body Quantum Simulations of Functionalized Structures"

Principal Investigator: Shiwei Zhang, College of William and Mary
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Henry Krakauer, College of William and Mary
Gustavo Scuseria, Rice University
Cyrus Umrigar, Cornell University

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **23,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (23,000,000 processor hours)

Research Summary:
The project describes an ambitious set of calculations in two areas: quantum chemistry for energy-related and magnetic materials, and cold atoms in optical lattices in atomic, molecular, and optical (AMO) physics. If successful, the effort will lead to the solution of longstanding challenges in accurately predicting key properties of these systems. It will also provide significant benchmark results for future simulations, experimental studies, and technological applications.

We have chosen the problems in these two areas to create synergy. They have great commonality in the requirement of high accuracy to resolve small energy differences and quantum states. They are also complementary: the quantum chemistry calculations emphasize the ability to treat materials-specific characteristics reliably and precisely, while the optical lattice calculations allow model engineering in which the many-body effects can be magnified to generate exotic new physics and chemistry. The same simulation approach will be used and was made possible by recent advances in the auxiliary-field quantum Monte Carlo method. The two areas will provide a wider span in testing the capability for precision many-body quantum simulations. Accurate treatment of such systems is a grand challenge in modern science. The combination of methodological developments and the advent of petaflop computing (and beyond) presents a unique and outstanding opportunity now to make fundamental progress.

Type: Renewal
Title: "Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations"

Principal Investigator: Jeffrey Greeley, Argonne National Laboratory
Co-Investigators: Thomas Bligaard, Technical University of Denmark
Jens Jørgen Mortensen, Technical University of Denmark
Jens Nørskov, Technical University of Denmark
Kristian Thygesen, Technical University of Denmark

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
The project's work for 2012 will continue fundamental studies of the size-dependent properties of metal nanoparticles in the nonscalable nano regime. This size range, in which nanoparticles' properties change in a manner that cannot be extrapolated from less computationally demanding bulk or single crystal surface calculations, is known to exhibit rapid, size-dependent property changes for a variety of applications. To understand variations in electronic and catalytic properties in this regime, it is essential to perform accurate first-principles calculations.

These calculations, which will ultimately assist in the design of enhanced nanocatalysts, are the continuing focus of this proposal. Researchers will continue to make use of GPAW, their highly scalable, $O(N^3)$, real space, and grid-based Density Functional Theory (DFT) code, for nanocatalytic modeling efforts. To date, they have determined changes in key thermodynamic parameters relevant to the oxidation of carbon monoxide, a classic reaction in heterogeneous catalysis, on gold (Au) nanoparticles ranging in size from 13 to 1,415 atoms. In addition, they have established that the size-dependent trends for Pt differ from Au particles in significant ways and are analyzing the electronic structure of Pt systems to understand these results. Building upon the analyses from last year, they will introduce both stoichiometric and reduced TiO_2 oxide supports into their calculations. These supports can have a significant impact on metal nanoparticles' catalytic properties, but limitations in computational resources have prevented researchers from understanding the detailed effect of these supports. The net result of these new studies will be a comprehensive, first principles-based picture of how the catalytic and electronic properties of oxide-supported metal nanoparticles evolve from the properties of molecular-like metal clusters to those of bulk-like metal surfaces.

Type: Renewal
Title: "Protein-Ligand Interaction Simulations and Analysis"

Principal Investigator: T. Andrew Binkowski, Argonne National Laboratory
Co-Investigators: Ian T. Foster, Argonne National Laboratory
Andrezj Joachimiak, Argonne National Laboratory
Benoît Roux, University of Chicago
Michael J. Wilde, Argonne National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **10,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
Improvement in predicting the ability of small molecules to bind to proteins can further basic knowledge in human health and holds the promise for improved processes in drug discovery. However, the success rate for docking has been mixed historically. Many of the shortcomings point to the scoring functions and the approximations and heuristics necessary to make the run-time feasible. The vast computing resources available now remove some of these constraints, allowing more advanced physics-based methods to be studied. Implementing these methods and making them more accessible to researchers helps to realize more of the promise that molecular simulation holds.

Using the advanced Blue Gene/P system, researchers are conducting a comprehensive analysis of protein binding domain and small molecule interactions through an automated system, including receptor analysis, protein-ligand docking, and binding free energy calculations. In addition, the team is performing the first, large-scale study of the computationally intensive FEP/MD-GCMC methodology for estimating free binding energy. Finally, in collaboration with the Center for Structural Genomics of Infectious Diseases, the team is conducting computer-aided drug discovery on human pathogens. The predicted computational results will be experimentally tested in binding assays and X-ray crystallography experiments, allowing for the important validation step necessary to evaluate the predictive power of biomolecular simulations.

In the next phase of the project, the team will use a production code to run protein-ligand interaction simulations on human pathogen targets of high biomedical value, such as *S. aureus* and *B. anthracis*. During 2012, the team will continue to operate the pipeline as originally designed regarding protein targets being studied. However, the team will begin to implement FEP calculations using NAMD, replacing the CHARMM-based calculations previously employed. They will also continue to work with biochemists and protein crystallographers to validate the computational predictions from their pipeline.

Type: New
Title: "Quantum Monte Carlo for Materials Design"

Principal Investigator: Tim Mueller, Massachusetts Institute of Technology

Co-Investigators: Jeffrey Grossman, Massachusetts Institute of Technology

Scientific Discipline: Materials Science: Materials Discovery, Design, and Synthesis

INCITE Allocation: **19,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (19,000,000 processor hours)

Research Summary:

Computational research has become an integral part of the materials design and development process. It is now possible to calculate property values for tens of thousands of materials, enabling high-throughput screening of materials and the generation of large data sets that can be mined to facilitate materials design. Such large-scale computational materials science is one of the cornerstones of the Materials Genome Initiative, a program recently unveiled by President Obama with the objective of leveraging information technology to dramatically accelerate the speed at which novel materials are brought to market.

The development of new materials can be significantly accelerated by enabling accurate predictions of whether or not a material is thermodynamically stable. For this reason a widely available, comprehensive database of accurate formation energies would significantly accelerate the materials design process. Because experimental data is only available for a small fraction of known materials and can be difficult to obtain, researchers frequently rely on density functional theory (DFT) calculations to provide formation energies. However DFT calculations can produce large errors in relative formation energies, especially when oxidation or reduction reactions are involved. Although it may be possible to develop methods to compensate for the error in DFT calculations, there is a lack of reliable benchmark data against which such methods can be calibrated.

This project will use quantum Monte Carlo (QMC) to calculate accurate formation energies for a set of 283 materials, consisting of 85 different elements in each of their most common oxidation states. In addition to providing valuable reference data against which other methods can be benchmarked, this project will form the foundation for a database that will grow to include accurate formation energies for all known materials, an invaluable resource for all materials researchers.

Type: Renewal
Title: "Quantum Monte Carlo Simulation of Models of Condensed Matter"

Principal Investigator: Richard Needs, University of Cambridge
Co-Investigators: Neil Drummond, University of Cambridge

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
Modeling the charge carriers in metals and semiconductors will help in understanding electronic devices. We will use the most accurate computational methods available to study the nature of the quantum mechanical states of these systems. Simulating strongly correlated quantum many-body systems on a computer is a grand-challenge problem of the first magnitude. Very high accuracy is required to resolve the tiny energy differences between competing phases. Simulation cells containing vast numbers of particles are required to allow the treatment of long-ranged correlation effects.

The questions we address in our research proposal are mostly related to the phase behavior and other properties of the homogeneous electron gas, which is our basic model of the charge carriers in metals and semiconductors. As well as improving our understanding of the electronic behavior of semiconductor devices with low carrier densities, the data we generate for the electron gas will benefit scientists using density functional theory (a simpler computational electronic structure method than quantum sMonte Carlo) to study the properties of more complicated systems.

Type: New
Title: "Quantum Monte Carlo Simulations of Light Elements at High Pressures"

Principal Investigator: David Ceperley, University of Illinois–Urbana-Champaign
Co-Investigators: Jeongnim Kim, University of Illinois–Urbana-Champaign
Miguel Morales, Lawrence Livermore National Laboratory
Carlo Pierleoni, University of L'Aquila, Italy

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **28,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (28,000,000 processor hours)

Research Summary:
This project will apply first-principles simulation methods based on quantum Monte Carlo and density functional theory to elucidate the equilibrium properties of hydrogen and other low-Z elements at high pressures.

The properties of dense hydrogen are important in astrophysics, for example in the understanding of the giant planets and the recently observed exoplanets. The equation of state of dense hydrogen is important for a wide range of technological applications such as for experiments conducted at the National Ignition Facility. What phase transitions dense hydrogen undergoes is a long-standing problem in condensed matter physics since Wigner and Huntington discussed it in 1935. However, for pressures greater than about 300 gigapascals, hydrogen's properties and even the underlying structures are not well understood.

The project will determine the ordering of the various crystal structures and their melting temperatures, and investigate whether liquid hydrogen could be stable at low temperatures. If so, it would have unusual properties due to the strong quantum effects of the ions. It will perform precise free-energy calculations and evaluate finite size effects and the quantum effects of both electrons and protons. It will also perform simulations of other low-Z elements, primarily helium and lithium. Under extreme compression, electron-core overlaps are expected to result in enhanced electron correlations. This work will test the validity of standard exchange-correlation approximations used in density functional theory for predicting properties of low-Z materials at extreme compression.

Type: Renewal
Title: "Scalable System Software for Performance and Productivity"

Principal Investigator: Ewing Lusk, Argonne National Laboratory
Co-Investigators: Pavan Balaji, Argonne National Laboratory
William Gropp, University of Illinois, Urbana-Champaign
Kamil Iskra, Argonne National Laboratory
Robert Latham, Argonne National Laboratory
Tom Peterka, Argonne National Laboratory
Robert Ross, Argonne National Laboratory
Han-wei Shen, Ohio State University
Rajeev Thakur, Argonne National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation: **5,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (5,000,000 processor hours)

Research Summary:
As hardware complexity skyrockets in high-end computing systems, it is not easy for applications to take complete advantage of the available system resources and avoid potential bottlenecks. The purpose of this project is to improve the performance and productivity of key system software components on these leadership-class platforms. Researchers are studying four different classes of system software: Message Passing Libraries, Parallel I/O, Data Visualization, and Operating Systems. They are using time on the platforms to understand and solve problems that occur at scale. The project team is leveraging their connections with software development groups in SciDAC, exascale codesign centers, and the larger community to most effectively address these challenges. Through rigorous experimentation, analysis, and design cycles, this project will dramatically improve the capabilities of not only systems being deployed in the near term, but of all systems pushing scalability limits in the near future.

Type: New
Title: "Simulation of Turbulent Lean Hydrogen Flames in High Pressure"

Principal Investigator: John Bell, Lawrence Berkeley National Laboratory
Co-Investigators: Marc Day, Lawrence Berkeley National Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **40,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (40,000,000 processor hours)

Research Summary:

One strategy for reducing US dependence on petroleum is to develop new fuel-flexible combustion technologies for burning hydrogen or hydrogen-rich fuels obtained from a gasification process. Fuel-flexible combustion systems based on lean premixed combustion have the potential for dramatically reducing pollutant emissions in transportation systems and heat and stationary power generation. However, lean premixed flames are highly susceptible to fluid-dynamical combustion instabilities making robust and reliable systems difficult to design. The goal of this proposal is to perform high-fidelity simulations of lean, premixed flames at high pressures. The focus of the simulations will be on hydrogen and hydrogen-rich fuels. High hydrogen content in the fuel introduces the potential for thermodiffusive instabilities, requiring that the simulations be performed with detailed chemistry and transport without the use of turbulence models.

Fuels that are rich in hydrogen are difficult to study. The high diffusivity of hydrogen causes the flames to burn in cellular structures, which have a distinctly different character than the "thin flame" approach that forms the basis for standard premixed flame theory. This has significant ramifications for theoretical studies, engineering design models, and even for the processing of experimental diagnostics. High-fidelity simulation with detailed chemistry and transport provides the only viable mechanism for obtaining a more detailed characterization. This is particularly true for high pressure flames where high-quality experimental measurements are very difficult to make. We plan a study of high-pressure lean premixed flames, focusing on hydrogen and fuels with a high hydrogen content. In the first year, we will consider flames in two idealized configurations, a planar flame propagating into homogeneous turbulence and the evolution of spherical flame kernels. In the second year, we will focus on modeling high pressure experiments performed using a low swirl burner. In the third year, we will extend those simulations to higher pressures characteristic of conditions in the combustion chamber of a stationary power-generation turbine. To capture the behavior of these types of flames, the simulations must incorporate detailed chemistry and transport and span a range of spatial scales needed to capture the range of turbulent scales characteristic of realistic flames.

Type: New
Title: "Simulation of Turbulent Multiphase Flows for Nuclear Reactor Safety"

Principal Investigator: Igor Bolotnov, North Carolina State University
Co-Investigators: Kenneth Jansen, University of Colorado–Boulder
Michael Podowski, Rensselaer Polytechnic Institute

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **14,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (14,000,000 processor hours)

Research Summary:
This project will perform direct numerical simulation of turbulent, bubbly, two-phase flows, allowing for an unprecedented level of detail and, potentially, answers to fundamental questions about the interaction between the bubbles and the liquid turbulence. Through these simulations, the project will collect statistical information about the turbulence parameters, such as turbulent kinetic energy and turbulent viscosity for an unprecedented Reynolds numbers for DNS simulations. This knowledge will allow assessment of theoretical knowledge about the turbulence spectrum for single-phase flows and provide new information about the bubble's influence on this spectrum, since no reliable data exists regarding the power spectrum law for two-phase turbulent flows.

Two subprojects will reproduce the experimental data for bubbly and annular flows to the highest level of detail. Major statistical parameters, such as flow rate, mean velocity, and gas volume fraction will be assessed against experimental data, while the higher-order statistics will bring new knowledge about two-phase flows, such as spectral information about gas/liquid interaction, bubbles, and droplets contribution to the turbulence. The third project will perform single and boiling two-phase flow simulations in pressurized-water nuclear reactor fuel bundles with complex geometry spacers.

Type: Renewal
Title: "Simulations of Deflagration-to-Detonation Transition in Reactive Gases"

Principal Investigator: Alexei Khokhlov, The University of Chicago
Co-Investigators: Joanna Austin, University of Illinois
Charles Bacon, Argonne National Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **20,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (20,000,000 processor hours)

Research Summary:
First-principles direct numerical simulations explain and predict high-speed combustion and deflagration-to-detonation transition (DDT) in hydrogen-oxygen gaseous mixtures. DDT and the resulting detonation waves in hydrogen may have especially catastrophic consequences in a variety of industrial and energy-producing settings, including the production, transportation, and use of hydrogen fuel, and safety of nuclear reactors, where hydrogen can be accumulated in cooling pipe systems due to radiolysis of water. First-principles simulations will be used to gain fundamental understanding of the physics of the strong, nonlinear, multiscale coupling of constituent combustion processes leading to DDT, and eventually for predicting the onset of detonation in DDT experiments and engineering devices.

Plans for the second year include: (A) Simulation of hot spot formation and autoignition behind reflected shocks to study autoignition mechanisms and validate simulations against ignition delay simulations. (B) Study of initiation of detonation by individual hot spots. (C) DDT simulations behind reflected shock. This will be used to study disruption of the flame by turbulence, formation, and detonation of nonuniform areas of reactivity. (D) Propagation and acceleration of a flame ignited at the closed end of the tube. This will study flame instabilities and development of boundary layers ahead of and behind the flame, as well as formation of shock waves propagating ahead of the flame front.

Type: Renewal
Title: "Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond"

Principal Investigator: Denise Hinkel, Lawrence Livermore National Laboratory
Co-Investigators: Peter Amendt, Lawrence Livermore National Laboratory
Bert Still, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **63,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (63,000,000 processor hours)

Research Summary:
In the 2010-2012 timeframe, Lawrence Livermore National Laboratory is tasked with achieving ignition at the National Ignition Facility (NIF). An important aspect of the ignition campaign is quantitative prediction of the level of laser backscatter in these targets. Understanding and mitigation of laser backscatter is important, as backscatter reduces the amount of input energy available for driving the fusion process. It can also alter implosion symmetry as well as preheat the ignition capsule via generation of hot electrons.

The NIF ignition campaign began in the late summer of 2009, and continues into 2012. In 2009, subscale targets, designed to emulate laser-plasma interactions (LPI) in ignition targets were fielded. The ignition campaign began in earnest in 2010, where ignition is sought using 1.2–1.8 MJ of input laser energy. It is also crucial to prepare for advanced target concepts beyond the ignition campaign, such as the Laser Inertial Fusion Engine (LIFE) concept that aims to provide high thermonuclear gain with mass-producible, low-cost targets. This project is performing simulations of laser propagation and backscatter in both ignition campaign and LIFE targets. Such simulations will generate scientific results that will have a major impact on the National Ignition Campaign and inertial fusion energy, as well as on the fundamental science of LPI.

Ideally, in 2012, the team will perform a pF3D simulation of the LIFE beams most at risk for LPI, and then look at kinetic effects with PIC simulations.

Type: New
Title: "Stochastic (w*) Convergence for Turbulent Combustion"

Principal Investigator: James Glimm, State University of New York at Stony Brook
Co-Investigators: Mirko Gamba, Stanford University
Xiangmin Jiao, State University of New York at Stony Brook
Johan Larsson, Stanford University
Xiaolin Li, State University of New York at Stony Brook
Parviz Moin, Stanford University
Vitali Morozov, Argonne National Laboratory
David Sharp, Los Alamos National Laboratory

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **35,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (35,000,000 processor hours)

Research Summary:
Large-eddy simulation (LES), the use of large-scale computing and complex probability equations to predict the turbulence of fluids, is an area of uncertainty in many engineering flow models. This project continues work on a stochastic convergence approach to reduce uncertainty in modeling turbulent combustion. It performs a verification simulation to test two fundamental ideas for numerical simulation of turbulent combustion: (1) finite-rate chemistry for LES, and (2) stochastic (w*) convergence based on probability distribution functions (PDFs) and mathematical ideas associated with Young measures. If the PDFs created by the simulation are found to display mesh convergence according to the w* definition, convergence properties will be identified and applications to key chemistry outputs such as heat release and species concentration explored.

Type: New
Title: "Studies of Large Conformational Changes in Biomolecular Machines"

Principal Investigator: Benoit Roux, University of Chicago / Argonne National Laboratory

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation: **18,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (18,000,000 processor hours)

Research Summary:
"Molecular machines" are complex macromolecular assemblies of proteins, nucleic acids, and carbohydrates that consume energy to perform specific biological functions. Their concerted action underlies all activities of a living cell. Presently, we know the shapes of several biological macromolecules in great atomic detail. Yet, these structures are insufficient to understand how a system can perform its function. For this, it is necessary to identify the different moving parts and understand how they act together to accomplish specific tasks. A good starting point is to characterize quantitatively how conformational and structural changes are associated with energetics. The free energy landscape, or potential of mean force, provides a powerful and unifying concept with respect to key parameters describing structural changes.

Molecular machines associated with biological membranes are particularly remarkable. Membrane-associated proteins play an essential role in controlling the bidirectional flow of material and information and as such are truly devices capable of complex tasks. These membrane-associated proteins include ion channels, transporters, pumps, receptors, kinases, and phosphatases. Some act as an electric switch, turned "on" and "off" by membrane voltage. Others, like the Src kinases, are turned "on" by phosphorylation, a chemical modification. Uncontrolled kinase activation is linked to a number of diseases, particularly cancer, making kinases important targets for therapeutic intervention. The Na/K pump, a large membrane protein transporting three Na+ outward and two K+ inward for each hydrolyzed ATP molecule, is critical: More than 40 percent of the energy produced in an animal cell is consumed by the Na/K ATPase to maintain Na+ and K+ gradients.

Like any machine, these proteins need to change shape and assume many conformational states to perform their functions. Our project is aimed at gaining a deep mechanistic perspective on membrane protein function, linking structure to dynamics, by characterizing the free energy landscape that governs key functional motions. Within the unified computational perspective provided by free energy landscapes, membrane proteins of increasing complexity and size are considered.

Type: New
Title: "The Solution of Three-Dimensional PWR Neutronics Benchmark Problems for CASL"

Principal Investigator: Thomas Evans, Oak Ridge National Laboratory
Co-Investigators: Greg Davidson, Oak Ridge National Laboratory
Josh Jarrell, Oak Ridge National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **19,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (19,000,000 processor hours)

Research Summary:

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is developing a virtual reactor simulation toolkit designed to use leadership-class computing resources.

CASL's primary modeling and simulation science driver is to enable nuclear reactor power uprates, life extensions, and higher fuel burnup. These objectives have been codified in 10 challenge problems, five of which are operational and five of which pertain to safety. In order to solve these problems, the Advanced Modeling Applications focus area in CASL has defined a series of test problems that each physics component in the virtual reactor toolkit must solve. These range from single fuel pins to whole cores and include varying levels of multiphysics coupling. Each of these problems requires a neutronics code capable of performing three-dimensional flux calculations with axial variations and sub-pin resolution depletion. Additionally, multigroup cross-section generation must be provided over a wide range of group structures in order to test the energy fidelity required to obtain accurate solutions to the test problems.

The project will use the Denovo transport system to solve the defined CASL neutronics problems in preparation for full-system simulations that will take place in years four and five of the CASL project.

Type: Renewal
Title: "Three Dimensional Simulations for Core Collapse Supernovae

Principal Investigator: Anthony Mezzacappa, Oak Ridge National Laboratory
Co-Investigators: John Blondin, North Carolina State University
Stephen Bruenn, Florida Atlantic University
Christian Cardall, Oak Ridge National Laboratory
William Raphael Hix, Oak Ridge National laboratory
Jirina Stone, Oak Ridge National Laboratory
Eirik Endeve, Oak Ridge National Laboratory
Pedro Marronetti, Florida Atlantic University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **30,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (30,000,000 processor hours)

Research Summary:

Core-collapse supernovas are the death throes of massive stars. They are the single most important source of elements in the universe. Understanding how they occur is one of the crucial unsolved problems in astrophysics. The focus of this project is to perform multidimensional, multiphysics simulations of core-collapse supernovas in an effort to determine the supernova explosion mechanism.

This project will perform three-dimensional simulations to understand how stars more than ten times the mass of our sun die in catastrophic stellar explosions known as core-collapse supernovae. Core-collapse supernovae 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, three-dimensional, multi-physics events, but there are as yet no three-dimensional models of sufficient realism. This is a significant void in supernova theory. The simulations described here will begin to fill this void. These simulations will be the first three-dimensional 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 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.

Type: New
Title: "Toward Exascale Computing of Type Ia and Ib,c Supernovae: V&V of Current Models"

Principal Investigator: Don Lamb, University of Chicago
Co-Investigators: Alan Calder, State University of New York at Stony Brook
Sean Couch, University of Chicago
Benedikt Diemer, University of Chicago
Anshu Dubey, University of Chicago
Carlo Graziani, University of Chicago
Aaron Jackson, State University of New York at Stony Brook
George Jordan, University of Chicago
Rick Kessler, University of Chicago
Min Long, University of Chicago
Vitali Morozov, Argonne National Laboratory
Michael Papka, Argonne National Laboratory
Katherine Riley, Argonne National Laboratory
Dean Townsley, University of Alabama
Venkatram Vishwanath, Argonne National Laboratory
Daniel van Rossum, University of Chicago
Klaus Weide, University of Chicago

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **40,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (40,000,000 processor hours)

Research Summary:
This project continues a program of verification and validation of Type Ia supernova models. More 3-D simulations of the explosion phase will be performed, along with 2-D simulations of the radiation transfer phase, to determine which models – and which parameter values of the models – agree best with the observed properties of typical Type Ia supernovae. The objective of the program is to better understand these explosions, enabling astronomers to improve the accuracy with which these explosions can be calibrated as "standard candles." Improving the use of Type Ia supernovae as "standard candles" will make them better cosmic yardsticks for determining the properties of dark energy, which is causing the expansion of the universe to accelerate. Understanding dark energy ranks among the most compelling problems in all of physical science.

Type: Renewal
Title: "Towards Breakthroughs in Protein Structure Calculation and Design"

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation: **33,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (33,000,000 processor hours)

Research Summary:
The computational resources from this INCITE award are being applied toward high-resolution protein structure calculation, de-novo protein-protein interface design for therapeutic applications, and de-novo enzyme design for fixation of carbon-dioxide to create biofuels. While much progress has been made in protein structure modeling, the ability to sufficiently sample conformation space is still a limiting factor for many protein-modeling applications: notably, protein structure prediction and design.

The broader impacts of this project will include pressing issues in the 21st century, among them deciphering the structures and functions of the vast number of protein sequences generated in current high-throughput sequencing projects and reducing the CO_2 levels in the atmosphere through enzymes designed to fixate CO_2 into industrially useful products.

Researchers will continue to develop the new parallelized version of the Rosetta de novo structure prediction method and transition their applications to the new algorithm. It should be noted that the new algorithm typically uses > 2K cores, while the previous version of Rosetta often used < 2K cores per simulation.

During 2012 researchers also intend to test how general the newly developed approach is for the design of protein binders. To that end, they have projects involved in targeting specific patches on proteins useful for diagnostics for tuberculosis (ACP2 from Mtb), as purification aids for human antibodies (protein A epitope on human IgG), as new diagnostics for malignant transformations (targeting the epidermal growth factor receptor), and for laboratory reagents that can target and disrupt oncogenes thought to be crucially important for cancer malignancy.

Type: New
Title: "Towards the Phase Diagram of Water and Ice with Quantum Monte Carlo"

Principal Investigator: Dario Alfè, University College London
Co-Investigators: Mike Towler, University of Cambridge
Wissam Al-Saidi, University of Pittsburgh
Michael Gillan, University College London
Kenneth Jordan, University of Pittsburgh
Michaelides Angelos, University College London

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **23,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (23,000,000 processor hours)

Research Summary:
Water is one of the most important substances on Earth, being crucial in fields ranging from biology to the Earth sciences, environmental sciences and medicine. The interaction of water molecules with various surfaces is an outstandingly important issue, as almost any surface in contact with the atmosphere is covered with at least a thin film of water molecules. Because of its importance, water is also one of the most studied substances, with early attempts to simulate its properties dating back nearly 80 years.

However, it is fair to say that the state of the art in computer simulation is still not sufficiently accurate. In particular, even seemingly simple properties like the diffusion coefficient, or the room pressure/temperature density, are difficult to calculate even with modern techniques based on density functional theory (DFT) with sophisticated exchange-correlation (XC) functionals including exact exchange and/or empirical van der Waals interactions. Our INCITE 2010 and 2011 projects have shown how quantum Monte Carlo (QMC) techniques can efficiently exploit petascale resources, and provide the much needed accuracy for water's interaction with various surfaces.

The crystalline phases of ice provide an excellent platform to assess and quantify the importance of weak van der Waals and hydrogen bond forces by presenting a large variety of distinct fixed geometries, with experimental data available for a number of properties including structural data and the cohesive energies of the various phases. Comparing cohesive energies and structural data obtained with QMC will provide a stringent test for the accuracy of the method, and early results obtained during this project's 2010 and 2011 projects are very encouraging, showing that QMC is able to achieve much better than chemical accuracy. The techniques to be applied are completely general, and the project's work will raise awareness of what it is possible to do with QMC methods on machines like Jaguar, which will become increasingly available in the future.

Type: Renewal
Title: "Turbulent Heating of Astrophysical Plasmas"

Principal Investigator: Gregory Howes, University of Iowa
Co-Investigators: William Dorland, University of Maryland

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **18,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (18,000,000 processor hours)

Research Summary:
Kinetic plasma theory is notoriously complicated, involving a huge range of spatio-temporal scales. With current resources, it is not possible to simulate or understand kinetic plasma turbulence in general. Fortunately, there are astrophysical and space plasma contexts for which a reduced kinetic theory is appropriate—*gyrokinetics*. Developed in the magnetic confinement fusion program over thirty years, gyrokinetics is the rigorous kinetic theory of magnetized, low-frequency plasma turbulence (low compared to the ion cyclotron frequency). Under appropriate conditions, all faster phenomena can be rigorously averaged, leaving one with a reduced (but still fully nonlinear) kinetic description of turbulence, instabilities and anomalous heating processes.

The goal of this project is to employ gyrokinetic theory, an elegant and efficient theoretical framework, in conjunction with the most powerful computational resources available, to investigate the dissipation of turbulence in astrophysical plasmas and determine the resulting plasma heating, a key problem in space physics and astrophysics. Our proposal aims to run a suite of first-principles, kinetic turbulence simulations of astrophysical turbulence over the dissipative range of scales from the ion Larmor radius to the electron Larmor radius. These simulations, using the high-performance parallel gyrokinetic simulation code AstroGK, aim to resolve the kinetic mechanisms responsible for the dissipation of turbulence in a weakly collisional plasma, leading the way for the development of the theoretical models of kinetic turbulence, enabling direct quantitative comparisons with observations, and providing the data necessary to characterize the resulting plasma heating.

Type: New
Title: "Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability"

Principal Investigator: Sanjiva Lele, Stanford University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **20,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (20,000,000 processor hours)

Research Summary:

Richtmyer-Meshkov instability (RMI) occurs when a shock wave interacts with a perturbed interface, separating fluids of different densities. After the shock refracts through the interface, perturbations grow; if the incoming shock is strong enough, or if the interface is sufficiently perturbed, the instability evolves into a turbulent mixing region. Even though Richtmyer-Meshkov instability occurs in a wide range of flows (e.g., supernovae explosions, inertial confinement fusion, and hypersonic propulsion systems), the turbulent mixing is not well understood. Few investigations of this phenomenon have been carried out, chiefly because of the unavailability of experimental data to validate numerical results, inadequacy of numerical algorithms, and the unknown (and possibly prohibitive) computational cost. Leveraging the IBM Blue Gene/P's capabilities, researchers are studying the fundamental physics governing this phenomena, in particular the mechanisms at play in turbulent multi-material mixing in shock accelerated flows. The study employs a novel solution-adaptive numerical framework that scales well and will enable scientific discovery through high-performance computing.

This study enables robust, high-fidelity simulations of the turbulent multi-material mixing generated after RMI. Computing these turbulence statistics, researchers will be able to answer fundamental questions such as: Is the classical Kolmogorov theory for turbulence valid in a transient non-stationary flow? How anisotropic is the turbulence generated in such problems? Does it relax toward isotropy? Is the inertial scaling for the decay rate in the energy-cascade a central element of turbulence modeling even valid in turbulent flows generated by the RMI?

High-resolution simulations of this phenomenon will capture the scales at which viscous dissipation and molecular mixing occur while representing the nonlinear dynamics of the energy-containing scales. The resulting database will enable a fundamental study of the mechanisms at play in turbulent multi-material mixing in shock-accelerated flows and help develop improved models for engineering.

Type: Renewal
Title: "Ultrascale Simulation of Basin-Scale CO2 Sequestration in Deep Geologic Formations and Radionuclide Migration using PFLOTRAN"

Principal Investigator: Peter Lichtner, Los Alamos National Laboratory
Co-Investigators: Glenn Hammond, Pacific Northwest National Laboratory
Richard Mills, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Environmental Sciences

INCITE Allocation: **19,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (19,000,000 processor hours)

Research Summary:
This project brings petascale computing resources to bear on current environmental problems involving global warming and sequestration of green house gases such as CO_2 in deep geologic formations and migration of radionuclides from highly contaminated DOE legacy sites from the WW-II and the Cold War. We propose to apply petascale computing to extreme scale problems involving CO_2 sequestration in large geologic basins to investigate the effects of displacing deep formation water brines by large volumes of CO_2 on potential contamination of drinking water aquifers.

In addition, we propose to apply petascale resources to uranium migration at the Hanford 300 Area. New data for stratigraphy, heterogeneity, and chemical processes are becoming available as part of an on-going DOE/IFRC project focused on the 300 Area, and we plan to incorporate this information into a larger revised site model. To minimize effects of inland boundary conditions on the local flow field, we plan to extend the domain away from the Columbia River increasing domain size and requiring increased resources over the current 4096 cores currently being used. Finally, at the Oak Ridge IFRC site, we will assist members of the ORNL IFRC project in constructing a watershed scale groundwater model with refined resolution using high performance computing for the S-3 and Y-12 sites. This model will integrate multiple processes at multiple scales into the model to investigate the influence of process interactions at small scales on the fate and transport of contaminants in the field, and the scale dependency of the controlling parameters such as dispersivity, attenuation, mass transfer and reaction rates. The calculations planned for this INCITE allocation will be the largest groundwater simulations ever carried out to date.

Type: Renewal
Title: "Unraveling the Physics of Magnetic Reconnection with 3D Kinetic Simulations"

Principal Investigator: William Daughton, Los Alamos National Laboratory
Co-Investigators: Vadim Roytershteyn, Los Alamos National Laboratory
Homa Karimabadi, University of California, San Diego

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **37,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK6 (37,000,000 processor hours)

Research Summary:
Magnetic reconnection is a fundamental plasma physics process that converts magnetic energy into particle energy and plays a critical role in a variety of physical environments such as planetary magnetospheres, solar flares, laboratory fusion experiments, and astrophysical plasmas. Despite over ~50 years of study, there are many important details that are not well understood.

With the advent of petascale computing and the new kinetic particle-in-cell code (VPIC) designed to exploit these machines, we are now able for the first time to conduct a systematic study to address some of the key issues in 3D kinetic reconnection. We have recently employed these capabilities to perform simulations ~100x larger than was previously considered state-of-the-art, with up to ~1.3 trillion particles. These powerful new capabilities are allowing us to address two important issues which may drastically alter previous 2D theories and simulations results. First, our preliminary results suggest that reconnection layers with a finite guide field may involve dynamical features that are inherently 3D, consisting of the continuous formation and interaction of flux ropes over a range of oblique angles. There are indications this may lead to a fully turbulent scenario in large systems. Second, we are now able to directly simulate the influence of current driven instabilities on the structure and time evolution of reconnection layers, and our preliminary 3D results indicate that electromagnetic modes in the lower-hybrid range can vigorously distort the electron current sheet for reconnection layers relevant to both space and laboratory plasmas. Our planned simulations on Jaguar will allow us to perform sophisticated validation comparisons of these results with the controlled laboratory reconnection experiment MRX at Princeton. The results will not only lead to a major advance in theoretical understanding of magnetic reconnection, but will also have impact in a variety of fields including space physics, solar physics, laboratory plasmas, and astrophysics.

Type: Renewal

Title: "Vibrational Spectroscopy of Liquid Mixtures and Solid-Liquid Interfaces"

Principal Investigator: Giulia Galli, University of California–Davis
Co-Investigators: Francois Gygi, University of California–Davis
Detlef Hohl, Shell International Exploration and Production
Leonardo Spanu, University of California–Davis

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **25,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (25,000,000 processor hours)

Research Summary:
Understanding pure water is an essential prerequisite for understanding the behavior of the liquid interacting with naturally occurring compounds such as carbon dioxide or methane.

The use of INCITE resources has been instrumental in assessing the accuracy of first principles theories for water. With an earlier INCITE allocation, several accurate flavors of density functional theory (PBEO and van der Waals functionals) were used to investigate water and ions in water with atomistic resolution. Specifically, researchers carried out *ab initio* molecular dynamics calculations using the massively parallelized density functional theory code Qbox on the IBM Blue Gene/P, and determined the structural and vibrational properties of liquid water for several temperatures. Calculations based on hybrid functionals (in particular, PBE0) yielded substantially improved results compared to those based on semi-local functionals (e.g., PBE). In particular, there is a dramatic improvement in the description of infrared spectra. These important findings suggest that through the use of high-performance computing, researchers can improve the description of aqueous environments.

Researchers will now carry out large-scale simulations and compute several properties of water and aqueous solutions at ambient conditions and under pressure. Using PBE0, the researchers are extending their investigation towards solvation properties of negative ions, such as chloride and sulfate, and mixtures of water with methane or carbon dioxide.

The researchers' work will play a key role in understanding the physical and chemical problem of processes involved in carbon-bearing fluids in the deep Earth, in particular, methane dissociation under upper mantle conditions, as well as in understanding structure and dissociation of water in contact with solid hydrophobic and hydrophilic surfaces.