Type: New
Title: "Advanced Reactor Thermal Hydraulic Modeling"

Principal Investigator: Paul Fischer, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Nuclear Energy

INCITE Allocation: **32,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (30,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (2,000,000 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 reactors. One of the active areas of research is in 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 the areas of interest and the thermal-hydraulic performance—pressure drop and mixing induced by the coolant flow—figures prominently in design questions.

Type: Renewal
Title: "Assessing Transient Global Climate Response Using the NCAR-CCSM3: Climate Sensitivity and Abrupt Climate Change"

Principal Investigator: Zhengyu Liu, University of Wisconsin–Madison
Co-Investigators: David Erickson III, Oak Ridge National Laboratory
Bette Otto-Bliesner, National Center for Atmospheric Research
Robert Jacob, Argonne National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **5,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (5,000,000 processor hours)

Research Summary:
This project will complete the first set of synchronously coupled transient ocean-atmosphere dynamic vegetation global climate model simulations of the past 21,000 years. In comparison with proxy climate records of the last 21,000 years, these experiments will significantly enhance our understanding of the transient response of the Earth system to different climate forcings. The project's experiments will address three fundamental questions related to future climate changes:

- What is the sensitivity of the climate system to different climate forcings, especially the greenhouse gases?
- How does the climate system exhibit abrupt changes on decadal/centennial time scales?
- What are the dominant mechanisms for climate response and climate change?

Type: Renewal
Title: "BG/P Plan 9 Measurements on Large Scale Systems"

Principal Investigator: Ronald Minnich, Sandia National Laboratories
Co-Investigators: David Eckhard, Carnegie-Mellon University
Charles Forsyth, Vita Nuova
James McKie, Bell Laboratories
Eric Van Hensbergen, IBM

Scientific Discipline: Computer Science

INCITE Allocation: **1,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (1,000,000 processor hours)

Research Summary:
This project will provide a new software environment for supercomputers that makes the supercomputer appear to be part of the user's desktop system, instead of a remote and hard-to-access external computer. Initial work will expand on the version of Plan 9 that was ported onto BG/L for the FASTOS program by SNL, Bell Labs, IBM, and Vita Nuova. Because the Plan 9 operating system was built with networks in mind, it requires less system administration support than other operating systems. In Plan 9's environment, files and directory trees can be imported from other machines, and with all resources defined as files or directory trees, sharing resources is greatly simplified. New drivers will be tested for the BG/P tree and torus networks. These new drivers make it possible for native file systems to use, e.g., the tree reduction network to make file systems very efficient. We plan to scale the Plan 9 implementation out to the full machine at ANL and measure performance for applications of interest. We will test all aspects of the Plan 9 environment and modify Plan 9 as needed for this large scale machine, in preparation for future systems with 10 million CPUs.

Type: Renewal
Title: "Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"

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

Scientific Discipline: Biological Sciences

INCITE Allocation: **25,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (25,000,000 processor hours)

Research Summary:

Efficient production of ethanol via hydrolysis of cellulose into sugars is a major energy policy goal. This project will perform highly parallelized multi-length-scale computer simulations to help understand the physical causes of resistance of plant cell walls to hydrolysis—the major technological challenge in the development of viable cellulosic bioethanol. The solution to this challenge may be the improvement of pretreatments or the design of improved feedstock plants (or both). Plant cell wall lignocellulosic biomass is a complex material composed of crystalline cellulose microfibrils laminated with hemicellulose, pectin, and lignin polymers. The simulations performed will be part of a larger effort to integrate the power and capabilities of the neutron scattering and high-performance computing facilities at Oak Ridge National Laboratory to derive information on lignocellulosic degradation at an unprecedented level of detail. The simulations will provide detailed knowledge of the fundamental molecular organization, interactions, mechanics and associations of bulk lignocellulosic biomass.

Type: Renewal
Title: "CHiMES: Coupled High-Resolution Modeling of the Earth System"

Principal Investigator: Venkatramani Balaji, National Oceanic and Atmospheric Administration (NOAA)/Geophysical Fluid Dynamics Laboratory (GFDL)

Co-Investigators: Tom Delworth, NOAA/GFDL
Isaac Held, NOAA/GFDL
Christopher Kerr, University Corp. for Atmospheric Research
Shian-Jiann Lin, NOAA/GFDL
Tony Rosati, NOAA/GFDL

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)

Research Summary:
Current resolutions of Intergovernmental Panel on Climate Change-class climate models are mostly in the 100-km range for both ocean and atmosphere. A central concern for the next generation of models is to understand natural and forced variability as we make the next leap in resolution. This leap is particularly interesting, as fundamental new physics appears in models of both atmosphere and ocean at the next step. In particular, we begin to see the influence of both ocean eddies and organized atmospheric storm systems at about 25-km resolution.

The Coupled High-Resolution Modeling of the Earth System (CHiMES) project proposes a series of long-term integrations involving a state-of-the-art coupled model of unprecedented resolution. Century-scale integrations of this model under varying initial conditions will provide valuable insights into the inherent predictability of this system, as well as statistically robust answers to key questions about the response of modeled tropical storm frequencies and intensity to climate change.

Type: Renewal
Title: "Clean and Efficient Coal Gasifier Designs Using Large-Scale Simulations"

Principal Investigator: Madhava Syamlal, U.S. Department of Energy, National Energy Technology Laboratory

Co-Investigators: Aytekin Gel, ALPEMI Consulting, LLC
Thomas O'Brien, National Energy Technology Laboratory
Sreekanth Pannala, Oak Ridge National Laboratory
Ramanan Sankaran, Oak Ridge National Laboratory
Chris Guenther, National Energy Technology Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **6,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (6,000,000 processor hours)

Research Summary:
This project will use large-scale parallel computing to speed up high-fidelity coal gasifier simulations, making such studies feasible for the ongoing design and optimization of advanced fossil fuel plants. Through use of MFIX, a multiphase computational fluid dynamics model, researchers will explicitly address the issue of scale-up by studying the effect of various operating conditions on the performance of a commercial-scale Clean Coal Power Initiative (CCPI) transport gasifier. The calibrated gasifier model is now being used to help with the design of commercial-scale systems intended for CCPI projects and tomorrow's zero-emissions fossil fuel plants. These high-fidelity simulations will provide design engineers with unique and valuable information on the gas and coal flow in the gasifier, information otherwise unavailable to them, since no experimental measurements or visualizations exist for the gasifier operating conditions. Furthermore, these simulations can help minimize the uncertainty in other scale-up issues, such as reactor length over diameter ratio, coal feed rate, solids recirculation rate, and effect of recycled gas. This is a unique and tremendous opportunity—the results of this project will have direct impact on the design of advanced, environmentally friendly power plants of the 21st century.

Type: Renewal
Title: "Climate-Science Computational End Station Development and Grand Challenge Team"

Principal Investigator: Warren Washington, National Center for Atmospheric Research

Co-Investigators:
David Bader, Oak Ridge National Laboratory
Lawrence Buja, National Center for Atmospheric Research
Phillip Cameron-Smith, Lawrence Livermore National Laboratory
Dave Considine, NASA Headquarters
John Drake, Oak Ridge National Laboratory
David Erickson, Oak Ridge National Laboratory
Steven Ghan, Pacific Northwest National Laboratory
James Hack, Oak Ridge National Laboratory
James W. Hurrell, National Center for Atmospheric Research
Philip Jones, Los Alamos National Laboratory
Robert Jacob, Argonne National Laboratory
Ruby Leung, Pacific Northwest National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **100,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (70,000,000 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. CCES will advance climate science through both an aggressive model-development activity and an extensive suite of climate simulations. Advanced computational simulation of the Earth system is built on the successful long-term interagency collaboration of NSF and most of the major DOE national laboratories in developing the Community Climate System Model (CCSM), together with NASA in carbon data assimilation, and efforts of university partners with expertise in computational climate research. 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 and is a principal focus of the CCES.

Type: Renewal
Title: "Computational Nuclear Structure"

Principal Investigator: David Dean, Oak Ridge National Laboratory
Co-Investigators: Hai Ah Nam, Oak Ridge National Laboratory
Witold Nazarewicz, University of Tennessee
Steven Pieper, Argonne National Laboratory
James Vary, Iowa State University

Scientific Discipline: Nuclear Physics

INCITE Allocation: **40,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (25,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)

Research Summary:
The nuclei located at the center of each atom comprise over 99.9 percent of the mass of the visible universe. This INCITE proposal spans computational methods that enable the study of all nuclei in pursuit of a modern understanding of nuclear structure, nuclear decays, and nuclear reactions. The theoretical description of all nuclei, which can be accomplished only through application of ultrascale computational capability, represents a major goal that could provide, for instance, an ab initio understanding of triple-alpha process — a set of nuclear fusion reactions by which a mature star creates carbon-12 nuclei from helium-4 nuclei - that is essential to life on Earth. The societal impact of understanding nuclei is far reaching, including energy, medicine, and global security and weapons applications, including stockpile stewardship. In all these areas, a high-quality nuclear-theory input is needed with quantifiable error bars.

Due to the wide range of nuclei, we employ several methods suitable for specific mass regions: light, medium, and heavy. This project uses ab initio techniques, including Green's Function Monte Carlo, no-core shell model, and nuclear coupled cluster methods, to calculate structural and reaction properties of light- and medium-mass nuclei, including two- and three-nucleon forces. The project also utilizes the Density Functional Theory to calculate properties of nuclei across the entire nuclear mass table. These DFT studies are necessary to predict nuclear properties relevant for the description of nuclear reactions, in particular neutron-nucleus reaction cross sections, and fission.

Type: Renewal
Title: "Computational Protein Structure Prediction and Protein Design"

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **50,000,000 Processor Hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (50,000,000 Processor Hours)

Research Summary:
The goals for this project are two-fold. First, high-resolution structure prediction tools will be used to build models of proteins with atomic-level accuracy; these will prove useful in rational structure-based drug design. Second, INCITE resources will be used to computationally engineer both proteins and enzymes with new functions for applications ranging from basic research to therapeutics to bioremediation. Prediction of high-resolution protein structures from their amino acid sequences and the refinement of low-resolution models to high resolution are longstanding problems in computational biology. Tools will be developed to help experimentalists solve structures of biologically important proteins for which experimental X-ray phases are not available or hard to obtain. In addition, early stage NMR structures will be refined to significantly speed up NMR structure determination. Many proteins carry out multiple complex cellular functions. In order to decipher which portions of the protein surface are responsible for a particular function, it would be desirable to selectively disable a portion of the protein surface. INCITE resources will be used to extend sampling, enabling researchers to test new protein scaffolds, examine additional structural hypothesis regarding determinants of binding, and ultimately design proteins that tightly bind endogenous cellular proteins. INCITE resources will also be used to computationally design a novel enzyme from de-novo methods to catalyze the carbamate hydrolysis reaction. A successful enzyme would enhance our understanding of mechanism of enzyme catalysis and offer potential avenues towards contaminated soil bioremediation. The creation of proteins capable of catalyzing any desired chemical reaction is a grand challenge for computational protein design.

Type: New
Title: "Computational Surface Science at High Accuracy with Quantum Monte Carlo"

Principal Investigator: Dario Alfè, University College London
Co-Investigators: Mike Gillan, University College London
Angelos Michaelides, University College London

Scientific Discipline: Physics: Condensed-Matter Physics

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)

Research Summary:
The binding of molecules to surfaces underlies an enormous number of important processes, including catalysis, corrosion, gas sensing, crystal growth, and many others. Computational modeling of these processes is crucially important in interpreting and guiding experiments, and in deepening understanding. But for many molecule-surface systems, the accuracy and realism of current methods often fall short of what is needed, and there is a very urgent need for techniques that can produce accurate benchmark values for key quantities such as molecule adsorption energies. This project shows how quantum Monte Carlo (QMC) techniques, implemented on petascale resources, enable this to be achieved. To demonstrate this, the project will produce very accurate binding energy curves for four exemplar systems: (i) water on graphite; (ii) water on the surface of magnesium oxide; (iii) water on the surface of sodium chloride; and (iv) carbon monoxide on the surface of copper.

The four exemplars chosen in this project will not only provide binding energy curves with unprecedented accuracy, but will stimulate the field of electronic structure theory to calculate binding energies with chemical accuracy in the multitude of other system where this is not just desirable, but very much needed to be able to solve important scientific and technological problems. The strength of the bonding of water on graphitic surfaces, an elusive quantity for both theory and experiments, is only one example. This stimulus toward a new era of computational physics is being opened by the combination of highly accurate QMC techniques and supercomputers like Jaguar, which are powerful enough to be able to use this technique with useful extensiveness.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: Renewal
Title: "Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz"

Principal Investigator: Thomas Jordan, Southern California Earthquake Center
Co-Investigators: Yifeng Cui, San Diego Supercomputer Center

Scientific Discipline: Earth Science: Environmental Sciences

INCITE Allocation: **27,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (7,000,000 processor hours)

Research Summary:
An interdisciplinary research team from the Southern California Earthquake Center will design, conduct, and analyze deterministic earthquake-wave-propagation simulations of large-scenario (Mw7.0+) earthquakes at frequencies above 1Hz on a regional scale. These simulations will utilize a realistic 3-D structural model of Southern California and will help geoscientists better understand earthquake-wave-propagation characteristics of large magnitude events in this region, including the duration and distribution of strong ground motions at frequencies of interest to civil and structural engineers. Large-scale, high-frequency simulations of scenario earthquakes are an essential tool for improving our understanding of the hazards and risks from potential future earthquakes, and the proposed simulations are of significant interest to the seismological, engineering, and emergency management organizations in California. The two primary goals for this work are to investigate the upper frequency limits of deterministic ground motion simulations and to better quantify how high-frequency seismic waves from large earthquakes contribute to the seismic hazard in Southern California and other regions.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: Renewal
Title: "Development and Correlations of Computational Tools for Transport Airplanes"

Principal Investigator: Moeljo Hong, The Boeing Company
Co-Investigators: John Bussoletti, The Boeing Company
Chen Chuck, The Boeing Company

Scientific Discipline: Engineering

INCITE Allocation: **6,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (6,000,000 processor hours)

Research Summary:

The project's main objective is to demonstrate the applicability and predictive accuracy of computational fluid dynamics (CFD) in a commercial airplane production environment. It will focus on validations of our CFD tools with known experimental data, as well as testing of new methodology before deployment for production use. This project will enable us to shorten the flow time required to accomplish the necessary simulations to demonstrate our goals. It allows more detailed components, more detailed physics, and more simulations to be included in the computation-result databases.

The project will focus on several aspects of airplane aerodynamics, including (but not limited to) unsteady validations of established experimental data, unsteady simulations of thrust reversers to enhance predictive accuracy, a study of grid convergence on a common-research model (CRM) for the 2009 American Institute of Aeronautics and Astronautics (AIAA) Drag Prediction Workshop, exploration of new processes based on an unstructured-grid Navier-Stokes solver for both transonic and high-lift (landing and takeoff) transport configurations, a study of wind tunnel walls and mounting bracket and struts interference and ground effects, transition model and its effects on transonic wing loading, and mesh adaptation for unstructured grids.

Type: Renewal
Title: "Electronic, Lattice, and Mechanical Properties of Novel Nano-Structured Bulk Materials"

Principal Investigator: Jihui Yang, General Motors Research and Development Center
Co-Investigators: Changfeng Chen, University of Nevada, Las Vegas

Scientific Discipline: Materials Science

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

Research Summary:
High-performance thermoelectric materials are essential components of automotive waste heat recovery technology. A successful technology development would save several hundred million gallons of gasoline annually. This project will address a key issue in the study of superior thermoelectric materials, the role of nanostructural features in the electronic, lattice, and mechanical properties of nanostructured bulk materials. (PbTe)1-x(AgSbTe2)x, one of the best intermediate-temperature thermoelectric materials, will be used as a model material system for this study. Lattice dynamics and stress-strain calculations will produce a phonon density of states and atomistic bond-breaking process of the materials, respectively, providing important insights into the mechanisms of the phonon scattering process, structural deformation, and failure modes.

Type: New
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 XT (9,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (1,000,000 processor hours)

Research Summary:
Currently, there is an intense research effort to use nanosystems for energy applications, including battery, solar cell, solar chemical cell, and thermoelectric cell. In this proposal, we will focus on nano solar cells. The goal is to understand the mechanisms of the critical steps inside a nano solar cell. These include 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. Answering these questions will not only help us to have a physical picture of how a nanosolar cell works, it will also enable us to calculate the efficiency for a given nano solar cell design, or to pinpoint the bottleneck of a device in order to design better solar cells. 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.

We have developed a series of simulation tools that enable us to study the above problems. All these are large-scale simulations, which can only be carried out using INCITE allocations on the leadership facilities.

Type: New
Title: "Gyrokinetic Simulation of Energetic Particle Turbulence in ITER Burning Plasmas"

Principal Investigator: Zhihong Lin, University of California–Irvine
Co-Investigators: Ronald Waltz, General Atomics

Scientific Discipline: Energy Technologies: Fusion Energy (Plasma Physics)

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)

Research Summary:
This project will conduct comprehensive simulations of energetic particle turbulence and transport in fusion plasmas. The confinement of energetic particles is critical for the burning plasma experiment ITER, since ignition depends on the balance between turbulent heat transport and self-heating by energetic particles produced by fusion.

The project will use two complementary global, nonlinear gyrokinetic codes: particle-in-cell GTC and continuum GYRO. Rigorous cross-code benchmarks between GTC and GYRO could provide verification of the gyrokinetic simulations. Comparisons with existing tokamak reactors, including the DIII-D tokamak dedicated experiments for energetic particle physics, will provide validations for the gyrokinetic simulations.

The proposed gyrokinetic simulations using GTC and GYRO will comprehensively assess the confinement properties of fusion products in ITER experiments. These simulations require the full power of petascale computers, with the GTC and GYRO codes making full use of the petascale system and incorporating important physics elements.

Type: Renewal
Title: "High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels"

Principal Investigator: Jacqueline Chen and Joseph Oefelein, Sandia National Laboratories

Co-Investigators: Jeffrey Doom, Sandia National Laboratories
Ray Grout, Sandia National Laboratories
Bing Hu, Sandia National Laboratories
Ahren Jasper, Sandia National Laboratories
Konstantin Kemenov, Cornell University
Stephen Klippenstein, Argonne National Laboratory
Guilhem Lacaze, Sandia National Laboratories
James Miller, Sandia National Laboratories
Stephen Pope, Cornell University
Edward Richardson, Sandia National Laboratories
Ramanan Sankaran, Oak Ridge National Laboratory
Donald Truhlar, University of Minnesota

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **67,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (65,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (2,000,000 processor hours)

Research Summary:
Transportation is the second-largest consumer of energy in the United States, responsible for 60% of our nation's use of petroleum, an amount equivalent to all of the oil imported into the United States. As our historic dependence draws to a close over the coming decades, new alternative fuel sources will emerge. Next-generation engines using alternative fuels are expected to be characterized by higher pressures, lower temperatures, and higher levels of dilution. They will operate fuel-lean in order to reduce energy consumption, pollutants, and greenhouse gas emissions. This multi-scale combustion project will use Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) techniques to perform high-fidelity simulations of the complex aero-thermo-chemical interactions typically encountered in internal combustion engines and quantum chemistry calculations of chemical kinetic parameters. Emphasis will be placed on fuel variability. DNS will be used to understand how jet flames in crossflow are stabilized, how thermal and composition stratification effects in kinetically controlled compression ignition combustion can be used to control the rate of combustion, and how intrinsic flame instability affects high pressure spherically expanding premixed flames. LES will be used to investigate turbulent reacting flow processes in an actual internal combustion engine geometry at the actual operating conditions, and underlying turbulence-chemistry interactions in laboratory-scale flames. The DNS and LES approaches are complementary. LES captures large-scale high-Reynolds-number mixing and combustion processes that occur over full engine-cycles, whereas DNS captures details of small-scale mixing and chemistry associated with combustion.

Type: Renewal
Title: "High-Fidelity Tokamak Edge Simulation for Efficient Confinement of Fusion Plasma"

Principal Investigator: C. S. Chang, New York University
Co-Investigators: Scott Parker, University of Colorado
Scott Klasky, Oak Ridge National Laboratory
Linda Sugiyama, Massachusetts Institute of Technology

Scientific Discipline: Physics

INCITE Allocation: **50,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (50,000,000 processor hours)

Research Summary:
Success of ITER and commercialization of the magnetic fusion reactors require good confinement of plasma energy at the plasma edge to form a plasma energy pedestal significantly above the cold, wall-interacting plasma of the "scrape-off" layer (this type of plasma operation is called "H-mode"). With the bifurcation of the edge plasma into the H-mode, the core plasma energy is quickly enhanced to the level of "fusion" condition for some unknown reasons. This is often called the "the-tail-wagging-the-dog" phenomenon in the fusion community. ITER program is based upon the H-mode pedestal formation and the-tail-wagging-the-dog phenomenon, both of which are not well understood. A first-principles understanding of these phenomena is one of the main mission of the present INCITE project.

Large scale simulations, pushing the limit of Jaguar, of tokamak plasma in realistic device geometries will be performed in this INCITE project. An extensive study of edge pedestal physics will be performed. In order to understand the nonlocal edge pedestal effect on the core plasma confinement, multiscale simulations of the whole volume plasma will also be performed. The whole volume includes the magnetic separatix, magnetic axis and the material wall boundary. Nonlocal turbulence propagation and the self-organization of the plasma profile to a critical global state will be simulated in H-mode plasmas. These simulations will hopefully shed lights to the understanding of the edge pedestal physics and the-tail-wagging-the-dog phenomenon, long awaited problems in magnetic fusion physics.

As the edge plasma pedestal becomes steeper, a large scale instability called "edge localized modes" (ELMs) crashes the plasma pedestal, limiting the core confinement and damaging the material wall. Control of large scale ELMs is an essential condition to the success of the ITER program. This INCITE will try to study what the edge localized modes are and how to control them.

Type: New
Title: "High Resolution Ensemble Simulations of Hurricanes"

Principal Investigator: Robert Gall, National Oceanic and Atmospheric Administration (NOAA)
Co-Investigators: Stan Benjamin, NOAA
Frank Marks, NOAA
Jeff Whitaker, NOAA

Scientific Discipline: Atmospheric Science

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)

Research Summary:
One of the highest priorities within the weather community is to improve our ability to forecast the track and intensity of hurricanes, with particular emphasis on lead times out to 4–7 days. In response, NOAA has created the Hurricane Forecast Improvement Program (HFIP) with the goal of improving forecasts of intensity and track by 20% within five years and 50% in ten years. These are very ambitious goals and probably can only be met using high-resolution (approximately 5–15 km) global atmospheric forecasting numerical models run as an ensemble. If the goals of HFIP can be achieved, the economic impact of an accurate 4–7 day forecast would be enormous. It would reduce the evacuation area required, reducing regional economic effects, and it would allow longer lead times for a more orderly evacuation of the areas impacted.

It is likely that high-resolution global ensembles will provide the necessary information for improving forecasts at the longer lead times, but this remains to be demonstrated. To demonstrate the value of this approach and to confirm whether this speculation is true, high-resolution global ensembles need to be run and verified. They also need to be run over enough cases such that the statistical significance of the skill of the forecasts can be determined. Generally this requires, at least, that every hurricane in a given season, and every forecast period from genesis to decay, be part of statistical evaluation of skill.

The project will run a high-resolution ensemble with 15-km horizontal resolution and 30 members (first year) and 10-km horizontal resolution and 26 members (second year) to better understand the global ensemble for forecasting track and intensity out to 7 days.

Type: Renewal
Title: "High Resolution Global Simulation of Plasma Microturbulence"

Principal Investigator: William Tang, Princeton Plasma Physics Laboratory
Co-Investigators: Mark Adams, Columbia University
Stephane Ethier, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **12,000,000 Processor Hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (12,000,000 Processor Hours)

Research Summary:

As the current global energy economy focuses on alternatives to fossil fuels, there is increasing interest in nuclear fusion, the power source of the sun and other stars, as an attractive possibility for meeting the world's growing energy needs. While progress has been impressive – leading to the international burning plasma experiment known as ITER, an outstanding problem is to minimize heat losses from such magnetic traps. Microturbulence is believed to be the primary mechanism by which particles and energy diffuse across the confining magnetic field in toroidal fusion systems. Understanding and possibly controlling the balance between these energy losses and the self-heating rates of the actual fusion reaction is key to achieving the efficiency needed to help ensure the practicality of future fusion power plants.

The "High Resolution Global Simulation of Plasma Microturbulence" INCITE project has utilized an advanced version of a gyrokinetic toroidal particle-in-cell code (GTC-P), which was derived from first-principles physics equations, to carry out realistic examinations of the effect of collisions on plasma confinement properties. Collisional dynamics were found to have a significant influence on the long-time behavior of turbulent plasmas and also to require a much larger number of particles to achieve the phase-space resolution needed. GTC-P, which now includes radial domain decomposition to greatly facilitate examining the key question of how plasma microturbulence properties might be affected as the plasma size increases from that of existing experiments to the future very large plasmas characteristic of ITER. In particular, it is now possible to efficiently examine the global turbulence properties in devices ranging from current scale experiments, which exhibit an unfavorable "Bohm-like" scaling with plasma size to the ITER scale plasma which is expected to exhibit a more favorable "gyro-Bohm" scaling of confinement. The code has now been optimized for use on the IBM Blue Gene/P quad-core Leadership Class Facility (LCF) at Argonne National Laboratory (ANL) to carry out these important and challenging advanced computational studies. With unprecedented resolution in a multi-dimensional phase-space, such advanced kinetic simulations have direct application to actual experimental devices, including the international ITER project, and give great promise of delivering scientific discoveries appropriate for "path to petascale" grand challenges.

Type: New
Title: "HPC Colony: Removing Scalability, Fault, and Performance Barriers in Leadership Class Systems through Adaptive System Software"

Principal Investigator: Terry Jones, Oak Ridge National Laboratory
Co-Investigators: Laxmikant Kale, University of Illinois–Urbana-Champaign
Jose Moreira, International Business Machines
Celso Mendes, University of Illinois–Urbana-Champaign
Esteban Meneses, University of Illinois-Urbana-Champaign
Yoav Tock, International Business Machines
Eliezer Dekel, International Business Machines
Roie Melamed, International Business Machines
Eli Luboshitz, International Business Machines
Menachem Shtalhaim, International Business Machines
Benjamin Mandler, International Business Machines

Scientific Discipline: Computer Science

INCITE Allocation: **4,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (4,000,000 processor hours)

Research Summary:
HPC Colony is a computer-science-oriented project focused on removing critical barriers that restrict computer-based scientific inquiry on future leadership-class machines. Unless these barriers are addressed, the breadth of applications capable of effectively using leadership-class machines will diminish due to increased demands placed on applications. Preliminary results have demonstrated computer science breakthroughs developed by Colony at scales up to 40,000-plus processor cores; this INCITE project is focused on advanced testing at leadership-class scales.

Our strategy for realizing these improvements in system software includes the use of three premiere applications: ChaNGA, OpenAtom, and NAMD. These three applications will be used to run larger problems and new science, thus furthering understanding in their respective domains.

Type: Renewal
Title: "An Integrated Approach to the Rational Design of Chemical Catalysts"

Principal Investigator: Robert Harrison, Oak Ridge National Laboratory
Co-Investigators: Roberto Ansaloni, Cray Europe
Djamaladdin Musaev, Emory University
Edoardo Apra, Oak Ridge National Laboratory
Carlo Cavazzoni, CINECA
Vincent Meunier, Oak Ridge National Laboratory
Bobby Sumpter, Oak Ridge National Laboratory
David Sherrill, Georgia Institute of Technology
William Shelton, Oak Ridge National Laboratory
William Schneider, University of Notre Dame
Steven Overbury, Oak Ridge National Laboratory
Mathew Neurock, University of Virginia
Duane Johnson, Emory University
David Dixon, University of Alabama
James Caruthers, Purdue University
Marco Buongiorno-Nardelli, North Carolina State University
A.C. Buchanan III, Oak Ridge National Laboratory
Jerzy Bernholc, North Carolina State University
Manos Mavrikakis, University of Wisconsin–Madison

Scientific Discipline: Chemistry

INCITE Allocation: **75,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (75,000,000 processor hours)

Research Summary:
Leadership-scale simulation using advanced theory in close collaboration with experiment is the only path toward the rational design of novel chemical catalysts that are crucial for many clean energy sources and for new manufacturing processes with improved activity and selectivity. Catalytic processes are directly involved in the synthesis of 20% of all industrial products. Within the DOE mission, catalysts feature prominently in cleaner and more efficient energy production, exemplified by the fuel cell and storage technologies required to realize the president's goal of a hydrogen economy. Experimental tools are unable to provide data on all of the steps involved in catalytic processes, especially under operating conditions. Computational modeling and simulation can fill this gap, supporting experiment by improved analysis and interpretation of data, and ultimately, in partnership with experiment, enabling the design of catalysts from first principles. Through a combination of leadership-scale computing and continued improvements in theory and algorithm, computational chemistry is about to cross a threshold that will deliver the 100–1000-times increase in effective simulation power required to make significant progress with our scientific objectives of improved activity and selectivity.

Type: Renewal
Title: "Interaction of Turbulence and Chemistry in Lean Premixed Laboratory Flames"

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

Scientific Discipline: Chemistry

INCITE Allocation: **8,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (8,000,000 processor hours)

Research Summary:
The FutureGen power plant project, sponsored by DOE's Office of Fossil Energy, is a near-zero-emissions combustion device designed to produce hydrogen and other synfuels from the gasification of coal and to sequester the carbon dioxide generated by the process. The fuels that result must then be burned in fuel-flexible combustion systems such as high-pressure gas turbines. Engineering design of such systems presupposes a fundamental understanding of combustion instabilities for ultralean premixed systems that simply does not yet exist. This project will use INCITE resources for a computational study to enable a fundamental understanding and characterization of thermo-diffusively unstable flames in both atmospheric and high-pressure regimes relevant to ultra-lean turbulent premixed burners. These are the unstable flames that will be key in the development of near-zero-emissions combustion devices. The simulations will provide details that are not directly accessible by experiment and will be used to validate interpretation of experimental data and to extend theoretical models of turbulence-flame interaction to include critical aspects of these flames not currently addressed. This has significant ramifications for theoretical studies, engineering design models, and even for the processing of experimental diagnostics.

Type: Renewal
Title: "Interplay of AAA+ Molecular Machines, DNA Repair Enzymes, and Sliding Clamps at the Replication Fork: A Multiscale Approach to Modeling Replisome Assembly and Function"

Principal Investigator: Ivaylo Ivanov, University of California–San Diego and Howard Hughes Medical Institute

Co-Investigators: John Tainer, Scripps Research Institute and Lawrence Berkeley National Laboratory
Xiaolin Chang, Oak Ridge National Laboratory
J. Andrew McCammon, University of California–San Diego and Howard Hughes Medical Institute

Scientific Discipline: Biological Sciences

INCITE Allocation: **4,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (4,000,000 processor hours)

Research Summary:
This highly interdisciplinary collaborative research is aimed at addressing critical problems in the biomedical arena and unified by the common theme of how cells accomplish faithful duplication of their genetic material.

Specifically, the project will focus on two areas: (i) function of sliding clamps and clamp-loaders within the replisome; and (ii) mechanisms of DNA repair enzymes. This research has direct bearing on understanding the molecular basis of genetic integrity and the loss of this integrity in cancer and in degenerative diseases, thus reflecting the priorities of federal agencies such as the NIH and the NSF. Furthermore, the fundamental biological mechanisms and the dynamic protein associations that form the subject of this proposal are conserved across bacterial, archaeal, and eukaryotic organisms and govern many metabolic processes occurring in response to environmental stress as the cells strive to regain homeostasis. Microbial genomes and metabolic responses to environmental stresses such as ultraviolet radiation, ionizing radiation, and oxydative stress are of direct relevance to the mission of DOE.

Type: New
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-Ii Lee, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **34,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (34,000,000 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 proposed 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: "Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles"

Principal Investigator: Christopher Wolverton, Northwestern University
Co-Investigators: Vidvuds Ozolins, University of California, Los Angeles

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

INCITE Allocation: **8,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (8,000,000 processor hours)

Research Summary:
General adoption of hydrogen as a vehicular fuel depends critically not only on the ability to extract it at sufficiently rapid rates but also on the ability to store hydrogen on-board at high volumetric and gravimetric densities. Recent experimental and theoretical studies have identified several new complex hydrides with thermodynamic properties and material storage capacities approaching and, in some cases, surpassing the DOE system targets. However, all these materials suffer from extremely poor kinetics. This project will use INCITE resources to rationally design novel nanostructured hydrogen storage materials with fast (de)hydrogenation kinetics and favorable thermodynamics. The accurate predictive power of first-principles modeling will be utilized to understand the microscopic kinetic processes involved in the hydrogen release and uptake so that we can design new systems with improved properties. Areas of study will include the fundamental factors that control hydrogen-metal bond strength, the role of surface structure and finite size on the thermodynamics and kinetics of hydride nanoparticles, and the effect of dopants and nanoscale catalysts in achieving fast kinetics and reversibility at the atomic level.

Type: New
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: **8,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (8,000,000 processor hours)

Research Summary:
Among all CFD methods, Large Eddy Simulation (LES) techniques have been the main scientific breakthrough of the past decade in the combustion community. They offer never before seen levels of precision but require significant computing power: in that sense, massively parallel machines are the real heart of LES for reacting flows. The objective of this proposal is to extend the computational capabilities deployed in previous studies of gaseous combustion to the combustion of liquid fuels in real gas turbines.

These studies will allow us to work on challenging issues encountered in the field of combustion and in gas turbine design such as atomization, breakup, and sprays. These issues are paramount if we wish to be able to fully understand what happens in airplane and helicopter engines allowing to advance towards the full numerical engine test bench; a virtual program able to assess the impact of any change any parameter on the combustion inside the engine such as replacing kerosene by a biofuel or modifying the injector of a combustor.

This proposal aims at removing a significant bottleneck: multiple groups in the USA and in Europe develop LES tools for reacting flow but most of them are limited to simple academic flows. Bringing the LES methodology to real combustion devices is a huge step in computing technology and modeling, this is the challenge of LETFLOC: Large Eddy Simulation (LES) of two phase flow combustion in gas turbines. All methods will be tested on real combustion chambers of gas turbines, using the full geometry and not one sector only as done today by all groups. The geometry will be obtained directly from engine manufacturers working with CERFACS. Thanks to the use of massively parallel computing, the work will focus on issues that have never been studied before because they are too expensive to address experimentally and were out of reach of computation until the last few years.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: Renewal
Title: "Large Scale Condensed Matter and Fluid Dynamics Simulations"

Principal Investigator: Peter Coveney, University College London
Co-Investigators: Steven Manos, University College London
Bruce Boghosian, Tufts University
Radhika Saksena, University College London

Scientific Discipline: Materials Science

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 will focus on the general theory of fluid flow in three diverse topics.

(i) Identification of Unstable Periodic Orbits (UPOs) in the Navier-Stokes equations:
The aim of our project in the field of turbulence research is to locate and characterize Unstable Periodic Orbits (UPOs) in turbulent hydrodynamics described by the Navier-Stokes equations. The UPOs provide us with an important characterization of the chaotic dynamics on the attractor of these systems. Indeed, it has been observed that a relatively small number of low-period UPOs may be used to calculate time/ensemble averages for chaotic dynamical systems from first principles. We aim to apply this observation to revolutionize the statistical prediction of turbulent fluid flows using a novel 4-dimensional approach that is parallel in space as well as in time.

(ii) Patient-specific whole brain blood flow simulations: Cerebral blood flow behavior plays a crucial role in the understanding, diagnosis and treatment of cardiovascular disease; problems are often due to anomalous blood flow behavior in the neighborhood of bifurcations and aneurysms within the brain. Simulation offers the possibility of performing patient-specific, virtual experiments to study the effects of courses of treatment with no danger.

(iii) Large scale molecular dynamics study of the materials properties of claypolymer nanocomposites. The objective of this work is to calculate the materials properties of clay platelets immersed in a polymer matrix (a nanocomposite system) which will facilitate the design of a wide range of environmentally beneficial functional materials for use across many industries, from automotive to the oil industry.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermi National Accelerator Laboratory
Co-Investigators: Michael Creutz, Brookhaven National Laboratory
John Negele, Massachusetts Institute of Technology
David Richards, Thomas Jefferson National Accelerator Facility
Stephen Sharpe, University of Washington
Claudio Rebbi, Boston University
Norman Christ, Columbia University
Richard Brower, Boston University
Robert Sugar, University of California, Santa Barbara

Scientific Discipline: Lattice Gauge Theory

INCITE Allocation: **107,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (67,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (40,000,000 processor hours)

Research Summary:
This project will deepen our understanding of the interactions of quarks and gluons, the basic constituents 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 Office of Science. INCITE resources will be used to generate gauge configurations with up, down and strange quarks on lattices that are sufficiently fine grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to the chiral and continuum limits. Three quark actions will be used in this work: clover, domain wall and improved staggered. Furthermore, we will validate calculations that cannot be checked through direct comparison with experiment, by performing them with more than one action. The gauge configurations will be used to determine a wide range of physical quantities of importance in high energy and nuclear physics: underlying parameters of the Standard Model of subatomic physics, including the masses of the quarks and the strong coupling constant and the elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix; and the mass spectrum of strongly interacting particles, including the baryon spectrum and photo-transitions in the charmonium sector.

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

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Paul Kent, Oak Ridge National Laboratory
Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **21,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (21,000,000 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: "Millisecond Molecular Dynamics of Chaperoning of Unfolded Polypeptide Chains by HSP70"

Principal Investigator: Harold Scheraga, Cornell University
Co-Investigators: Jozef Liwo, Cornell University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **6,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (6,000,000 processor hours)

Research Summary:
The dynamics of proteins and mechanisms of protein folding and unfolding play a fundamental role in biological processes such as enzymatic reactions, signal transduction, immunological response, cell motility, and also in diseases such as cancer and amyloid formation. The native three-dimensional structure of a protein is entirely encoded in its amino-acid sequence. However, in vivo folding is assisted by special proteins termed molecular chaperones. The 70-kDa heat- shock proteins (HSP70s) appear to be the ma jor chaperones involved in assisting correct folding of nascent and misfolded proteins and preventing their aggregation in the cytosol. They also inhibit programmed cell death (apoptosis) by interacting transiently with other proteins of the apoptosis pathways; this function is undesirable in cancer cells. Inhibition of the anti-apoptotic role of HSP70 and stimulation of its extra-cellular role in the immune response are two strategies used in the search for new cancer therapies and vaccines for infectious diseases.

The goal of this work is to determine, by means of large-scale coarse-grained simulations, the dynamics of the molecular HSP70 molecular chaperone and the dynamics of binding of a peptide substrate to it, in order to understand the mechanism of chaperone action. The HSP70s (70- kDalton heat-shock proteins) are essential molecular chaperones present both in prokaryotic and eukaryotic cells of all organisms. Because of their interactions with many proteins of the cell machinery, in particular in stress conditions, the HSP70s were found to be related to many diseases such as, e.g., oncogenesis, Parkinson disease, neurodegenerative diseases, obesity etc. Understanding the mechanism of substrate binding and release will provide the means of controlling these processes.

Type: Renewal
Title: "Modeling the Rheological Properties of Concrete"

Principal Investigator: William George. National Institute of Standards and Technology (NIST)
Co-Investigators: Nicos Martys, NIST
Judith Terrill (nee Devaney), NIST
John Hagedorn, NIST
Edward Garboczi, NIST

Scientific Discipline: Materials Science

INCITE Allocation: **2,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (2,000,000 processor hours)

Research Summary:
Understanding mechanisms for the dispersion or agglomeration of suspensions remains a great challenge and has technological application in a wide variety of areas, including the pharmaceutical, food, coatings and building industries. This project will study the flow of dense suspensions and related colloidal systems composed of rigid bodies, with and without interparticle interactions, having a wide range of size and shape, and under a variety of flow conditions such as shear and around obstacles. The computational approach is based on a modified Dissipative Particle Dynamics (DPD) model, which includes lubrication and Van der Waals forces for different shape particles near contact. Accounting for these broad size and shape variations along with strong interparticle forces is extremely demanding, computationally. The improved general understanding of rheological properties derived from this research should have a broad impact with results transferable to other complex fluid systems of interest such as nanoparticle systems.

Type: Renewal
Title: "Molecular Simulation of Complex Chemical Systems"

Principal Investigator: Christopher Mundy, Pacific Northwest National Laboratory
Co-Investigators: Roger Rousseau, Pacific Northwest National Laboratory
Allesandro Durioni, IBM Research-Zurich
Greg Schenter, Pacific Northwest National Laboratory
Shawn Kathmann, Pacific Northwest National Laboratory
Joost VandeVondele, University of Zurich

Scientific Discipline: Chemistry

INCITE Allocation: **12,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (10,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (2,000,000 processor hours)

Research Summary:
Moving molecular simulation forward beyond incremental steps requires a radically new simulation protocol. This project will apply the efficient sampling methods used with density functional-based interaction potentials to generate full elucidation of complex chemical processes that are vital to our future. INCITE resources will be used to develop new understanding of chemical reactions in solutions and at interfaces, especially as related to hydrogen storage and catalyisis. This research will establish the future protocol for the application of high-performance computing to present and future grand challenges in the chemical sciences. The synergy of molecular simulation with state-of-the-art hardware will keep the United States competitive in delivering future technologies.

Type: New
Title: "Multidimensional Models of Type Ia Supernovae from Ignition to Observables"

Principal Investigator: Stan Woosley, University of California–Santa Cruz
Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
John Bell, Lawrence Berkeley National Laboratory
Dan Kasen, University of California–Santa Cruz
Andy Nonaka, Lawrence Berkeley National Laboratory
Michael Zingale, Stony Brook University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **5,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (5,000,000 processor hours)

Research Summary:
Understanding how supernovae work has been a central problem in stellar evolution for at least 50 years and a robust problem in simulation for almost as long. Only recently have computers and codes been developed that are capable of definitive calculations. The convection and turbulence that occur in Type Ia supernovae (SNe Ia) require high-resolution three-dimensional simulations to capture the relevant physics. This is especially important in the convective phase, which is characterized by an astronomically large (10^{14}) physical Reynolds number that sets the initial conditions for the runaway. Flame-generated turbulence also plays a major role in determining the flame speed. While the project does not hope to attain the physical Reynolds number or resolve the flame width (10^{-3} cm in a star 2,000 km in radius), it is important to follow the convection deep into the turbulent regime and to carry at least one decade of resolution in the integral scale for the turbulence everywhere there is burning. No calculations have done this so far, let alone any survey of the expected variable conditions (ignition location, density, metallicity, detonation criterion, and carbon-oxygen ratio). Using codes and expertise developed with the support of the DOE Scientific Discovery through Advanced Computing program, the project will perform a series of calculations that will result in a transformational advance in our understanding of SNe Ia.

Type: Renewal
Title: "Multidimensional Simulations of Core Collapse Supernovae"

Principal Investigator: Anthony Mezzacappa, Oak Ridge National Laboratory
Co-Investigators: Jirina Stone, Oak Ridge National Laboratory
John Blondin, North Carolina State University
Stephen Bruenn, North Carolina State University
Christian Cardall, Oak Ridge National Laboratory
W. Raphael Hix, Oak Ridge National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **34,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (34,000,000 processor hours)

Research Summary:
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: "Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials"

Principal Investigator: Mark Jarrell, Louisiana State University
Co-Investigators: Zhaojun Bai, University of California–Davis
Eduardo D'Azevedo, Oak Ridge National Laboratory
Thomas Maier, Oak Ridge National Laboratory
Juana Moreno, Louisiana State University
Sergey Savrasov, University of California–Davis
Richard Scalettar, University of California–Davis
Karen Tomko, Ohio Supercomputer Center

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **17,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (17,000,000 processor hours)

Research Summary:
Petascale computing, combined with new formalism, algorithms, and codes, holds the promise of fundamental discovery in the study of complex correlated materials. Many technologically important materials display complex behavior due to strong electronic correlations. These include magnets, magnetoresistive materials, lanthanides, actinides, and high-temperature superconductors. An unbiased treatment of these phenomena requires an approach able to treat the correlations over all relevant length scales. First-generation numerical and analytical methods have, for example, lent qualitative understanding of the origins of superconductivity, the pseudogap, and of the segregation of spin and charge into striped patterns in heavy fermion and transition metal oxides. Yet these algorithms are fundamentally limited in their treatment of the different length scales and, therefore, have often employed approximations that introduce systematic biases in order to make progress.

The multiscale many body (MSMB) approach circumvents these problems by parsing correlations into different length scales and using an appropriate approximation for each. INCITE resources will be used to qualify the MSMB method and to study increasingly complex models of the cuprates and address problems of current interest, including the quantum critical point and its relationship to the superconducting dome at finite doping in the 2D Hubbard model. The MSMB method holds the promise to circumvent problems that have long inhibited the study of strongly correlated electronic systems, and these studies will increase our understanding of long-ranged correlations in strongly correlated systems.

Type: Renewal
Title: "Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence"

Principal Investigator: Susan Kurien, Los Alamos National Laboratory
Co-Investigators: Mark Taylor, Sandia National Laboratories
Ramesh Balakrishnan, Argonne National Laboratory
Leslie Smith, University of Wisconsin – Madison

Scientific Discipline: Engineering

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

Research Summary:
A focal point in the traditional approach to modeling large-scale atmospheric and ocean flows is the assumption of hydrostatic balance between the gravitational force per unit volume and the vertical component of the pressure gradient. The hydrostatic balance assumes that vertical accelerations are small compared to vertical pressure gradients and vertical buoyancy forces, which is a good approximation for quasi-geostrophic flows such as large-scale, vertical motions. However, the hydrostatic approximation is uncontrolled, valid only for variations in the horizontal direction that are large compared to the vertical height H of the domain. While it is very accurate over a large part of the ocean, the approximation neglects vertical overturning processes, such as convection, and therefore hydrostatic models require parameterizations in areas where such processes occur. These climate scale models are being applied more frequently to high-resolution regional modeling studies such as in the Gulf of Mexico and the Arctic basin. Regional models require very high resolution, on the order of a few kilometers or less, in order to resolve local topographic features. Therefore, they may violate the validity of the hydrostatic approximation so that the validity of the results and the extent of the inaccuracy involved is unknown.

Our purpose here is to quantify the behavior of rotating and stratified turbulent flows in which multiple time and spatial-scales may be simultaneously important, and for which non-hydrostatic effects are not negligible and a statistical description becomes necessary. These results would have a profound effect on our understanding of how ocean/atmosphere/climate models need to handle their fluid dynamics component, particularly when it comes to prediction of long-term phenomena such as the thermohaline circulation and climate-change. This work prepares the community for the next-generation of climate models which will need to account for the long-term consequences of non-hydrostatic effects.

Type: New
Title: "Overcoming the Turbulent-Mixing Characterization Barrier to Green Energy and Propulsion Systems"

Principal Investigator: Anurag Gupta, General Electric Global Research
Co-Investigators: Gregory Laskowski, General Electric Global Research
Hao Shen, General Electric Global Research
Chingwei Shieh, General Electric Aviation

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **19,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (19,000,000 processor hours)

Research Summary:
Research and development in simulation-based science has long formed a core component of General Electric's (GE's) technology base used to develop advanced energy and propulsion systems – ranging from wind turbines to gas turbines, diesel/hybrid engines to aircraft engines. Computational fluid dynamics (CFD) in particular has played a key role in the aerodynamic/ thermal/acoustic design of these products, from physical understanding to invention. As the demands for increased efficiency and power production combine with new emphasis on renewable power and lower emissions, traditional Reynolds-Averaged Navier Stokes (RANS) approaches are seen reaching their limit to accurately characterize key flow physics, specifically multi-scale, turbulent mixing in boundary layers and high temperature shear flows like jets and wakes.

With recent successes in proof-of-concept work using Large Eddy Simulation (LES) in these areas, and demonstrated massively parallel scalability on modern high-performance computing architectures, the GE Global Research team is proposing the first leg of a multi-year effort. This one-year effort will refine, validate and demonstrate the use of LES on real-world scale problems to accurately characterize – in detail or scope not possible via physical experimentation – key phenomena that have the potential to significantly impact efficient and environmentally friendly energy and propulsion systems. For a one-year INCITE allocation of 65.75 million CPU hours on the ALCF IBM B/G, three fundamental problems will be studied: wind turbine airfoil self-noise; heated jet noise; and film cooling heat transfer. The impact of higher-order statistics will be acquired via LES as a Numerical Test Facility to quantify the effect of trailing edge thickness on self-noise for modern, high-lift cambered wind turbine airfoils; density variations and Reynolds number scaling on heated jet noise for realistic engine-scale nozzles; and film cooling flow turbulence on heat transfer, jet-wake interaction, and vane wake evolution for high pressure turbines.

Findings from the proposed research will significantly improve the prediction models and design

capabilities for next-generation energy and propulsion systems.

Type: New
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
Bronis R. de Supinski, Lawrence Livermore National Laboratory
Jack J. Dongarra, University of Tennessee–Knoxville
William D. Gropp, University of Illinois–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–Madison
Leonid Oliker, Lawrence Berkeley National Laboratory
Allan Snavely, University of California–San Diego
Jeffrey S. Vetter, Oak Ridge National Laboratory
Katherine A. Yelick, University of California–Berkeley

Scientific Discipline: Computer Science

INCITE Allocation: **28,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (8,000,000 processor hours)

Research Summary:

To maximize the utility of Department of Energy leadership class systems such as the Cray XT4, Cray XT5, and IBM Blue Gene/P, 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. This proposal is for a performance community end station that will provide the required access.

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 BG/P and XT4/5, making these available to high-end computing users, and further develop the tools and middleware so as to take into account the scale and unique features of 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 candidate leadership class application codes, including development of new parallel algorithms.

Type: New
Title: “Petascale Adaptive Computational Fluid Dynamics for Applications with High Anisotropy”

Principal Investigator: Kenneth Jansen, Rensselaer
Co-Investigators: Chris Carothers, Rensselaer
Onkar Sahni, Rensselaer
Mark Shephard, Rensselaer

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **20,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (10,000,000 processor hours)

Research Summary:
This project will efficiently perform large-scale flow simulations of complex problems by adapting the grid to locally match the solution's highly anisotropic flow features. Reliable, automated techniques will be employed, and advanced further, to understand the complex flow physics yielding insight into open scientific questions such as active flow control for effective reactor design and modeling active flow control in synthetic jets.

Under this project a mature finite-element based flow solver (PHASTA) will be employed along with anisotropic adaptive meshing procedures to attack fluid flow problems where anisotropic solution features like strong boundary and shear layers can only be located and resolved through adaptivity. Furthermore, these flow problems not only involve complicated geometries such as human arterial system or detailed aerospace configurations, but also complex physics such as fluid turbulence and multi-phase interactions, resulting in discretizations so large that only a highly scalable, anisotropic adaptive flow solver capable of using massively parallel (petascale) systems will yield insightful solutions in a relevant time frame.

Type: Renewal
Title: "Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling"

Principal Investigator: Lie-Quan Lee, SLAC National Accelerator Laboratory
Co-Investigators: Zenghai Li, SLAC National Accelerator Laboratory
Kwok Ko, SLAC National Accelerator Laboratory
Andreas Kabel, SLAC National Accelerator Laboratory
Cho Ng, SLAC National Accelerator Laboratory

Scientific Discipline: Physics

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

Research Summary:
The International Linear Collider (ILC), a proposed electron-positron accelerator with an estimated cost of $6.75 billion, will be one of the world's largest, most complex, and most expensive scientific facilities. It opens the door to scientists to address many of the most compelling questions in the 21st century about dark matter, dark energy, and the fundamental nature of matter, energy, space, and time. The ILC consists of two main 14-km linear accelerators (main linacs) for accelerating electron and positron beams to 250 GeV. The main linacs constitute a substantial portion of the overall cost of the ILC. Thus, it is important to optimize the designs of the essential components of the linac to achieve prescribed operational requirements. This project will combine powerful and advanced simulation tools developed at SLAC with INCITE resources to simulate the RF unit, the basic accelerator section in the ILC main linacs, and to evaluate the effects of wakefields and heat loads by incorporating multiphysics analysis. These large-scale simulations will make a significant impact on ILC design, providing improved performance, increased reliability, and lower cost.

Type: New
Title: "Petascale Modeling of Nano-Electronic Devices"

Principal Investigator: Gerhard Klimeck, Purdue University
Co-Investigators: Benjamin Haley, Purdue University
Mathieu Luisier, Purdue University

Scientific Discipline: Materials Science: Nanoelectronics

INCITE Allocation: **18,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (18,000,000 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. The Non-Equilibrium Green's Function (NEGF) formalism has proven to be a powerful conceptual and computational framework for treating three-dimensional quantum transport in nanodevices. 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: New
Title: "Petascale Particle-in-Cell Simulations of Fast Ignition"

Principal Investigator: John Tonge, University of California, Los Angeles
Co-Investigators: Warren Mori, University of California, Los Angeles
Chuang Ren, University of Rochester

Scientific Discipline: Energy Technologies: Fusion Energy (Plasma Physics)

INCITE Allocation: **7,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (7,000,000 processor hours)

Research Summary:
Energy is the ultimate driver for economic growth and social development. Fusion energy is regarded one possible long-term energy solution for humanity that is environment friendly and safe. Fast ignition (FI) is a promising inertial confinement fusion (ICF) scheme to improve the viability of inertial fusion energy as a practical energy source. Unlike the conventional hot-spot ignition in ICF, this approach separates the compression of the fusion fuel from the ignition step. First, a compression laser compresses a spherical shell of deuterium-tritium ice to high density at low temperature, without a central hot spot. Then, a second very high-intensity laser delivers a pulse of energy that ignites the compressed fuel. Compared to hot-spot ignition, the FI concept promises much higher gain for the same driver energy and possible reduction of the driver energy necessary to achieve ignition. There is worldwide interest in FI and its associated science. Major experimental facilities are being constructed which will enable "proof of principle" tests of FI in integrated sub-ignition experiments, most notably at the OMEGA-EP facility in the USA and the FIREX facility in Japan.

The ignition phase determines the coupling of the ignition laser to the target core and thus the viability of FI. This phase is also the least understood one in FI. PIC methods provide the best-available simulation tool to understand the highly nonlinear and kinetic physics in the ignition phase. The proposed work covers much of the physics both the channel and cone guided schemes (channeling and hole-boring for the channel guided scheme, laser absorption, and electron transport up to moderate densities) with the goal to answer the following key questions. (1) Does the laser propagate adequately through the residual plasma in the channel or cone? (2) Does the laser hole-bore beyond the critical density? (3) What is the spectrum of the laser-generated energetic electrons at the laser-plasma interface and near the core? (4) What is the energetic electron transport process beyond the laser-plasma interface in plasma with densities up to 1,000-10,000 times the critical density? The proposed work will expand upon previous large-scale 2D PIC simulations on FI and move to 3D simulations where it is feasible.

Type: New
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: **8,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (8,000,000 processor hours)

Research Summary:
For the past 80 years, the tool of choice in experimental high-energy physics has been particle accelerators. The Large Hadron Collider (LHC) at the European Organization for Nuclear Research, or CERN, came online in 2008. The construction cost alone for the LHC machine is nearly $10 billion, and it is clear that, if the same technology is used, the world's next "atom smasher" will cost at least several times as much in today's dollars. 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: "A Petascale Study of Turbulent Mixing in Non-Stratified and Stratified Flows"

Principal Investigator: Pui-kuen Yeung, Georgia Institute of Technology
Co-Investigators: Diego Donzis, Texas A&M University
Dmitry Pekurovsky, San Diego Supercomputer Center
James Riley, University of Washington

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)

Research Summary:
Turbulence is a grand challenge problem in computational science well-recognized for its complexity (disorderly fluctuations over a wide range of scales in space and time) and environmental and technological importance in subjects such as atmospheric science, oceanography, pollution control, and energy efficiency. One of the most important properties of turbulence is efficient mixing, which occurs as velocity fluctuations break up macroscopic non-uniformities of momentum, temperature, chemical composition, humidity, salinity, etc. into smaller scales where molecular diffusion acts to smear out local gradients. Besides the Reynolds number, an important parameter is thus the ratio, called the Schmidt number, which is the ratio of kinematic viscosity to the molecular diffusivity of the diffusing substance or property. In many cases, difficulties faced by both numerical simulation and laboratory experiments in attaining truly realistic parameter regimes have made it difficult to compare results with field measurements and address current issues of controversy.

In this INCITE proposal, two ambitious simulations are planned of turbulent mixing at high Schmidt number, with and without density stratification, with as many as 64 billion grid points. These simulations will provide long-awaited answers on many important issues, such as viscous-convective and viscous-diffusive scaling ranges.

Contributions to the state of the art of large, communication-intensive user applications are expected to result from further optimization efforts. The project team will also work with other researchers in modeling, theory, and experiment in order to derive maximum benefit from huge databases to be generated through deployment of leadership-class petascale computing resources.

Type: New
Title: "Prediction of Bulk Properties Using high Accuracy Ab Initio Methods Interfaced with Dynamical Calculations"

Principal Investigator: Theresa Windus, Ames Laboratory
Co-Investigators: Brett Bode, University of Illinois
Mark Gordon, Ames Laboratory
Monica Lamm, Iowa State University
Michael Schmidt, Ames Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **8,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (8,000,000 processor hours)

Research Summary:
The focus of this proposal is on using high quality electronic structure theory, statistical mechanical methods, and massively parallel computers to address the prediction of bulk properties of water systems which require high fidelity. These molecular scale problems are of critical importance to national priority scientific issues such as global warming, the environment and alternative fuels. Many important problems in the chemical sciences are so computationally demanding that the only perceived option for addressing such problems is to employ low-level methods whose reliability is suspect. The electronic structure community has well established protocols for assessing the reliability of methods applied to small and medium systems; e.g., by employing increasingly sophisticated methods that are generally accepted to be reliable, and studying the convergence of the predictions. Such protocols have not been available for the very large systems that are typified by the three examples in the present proposal. A primary motivation for the research proposed herein is to ensure that reliable levels of electronic structure theory (e.g., many body perturbation theory and coupled cluster theory) can realistically be employed to solve challenging problems of national interest. The proposed research will accurately address extended systems whose sizes can only be addressed with massive computational resources.

The work in this proposal focuses on understanding the molecular level dynamics of water, the formation of aerosols important in cloud formation and the interactions of dendrimers with ligands of environmental importance. In each of these applications, the underlying research will set a new standard for the predictive computation of bulk properties. The two primary electronic structure codes to be used in these simulations are GAMESS and NWChem. These two codes are without question the two most broadly scalable electronic structure systems. Therefore, the impact of this research will be across a broad area of the chemical sciences and will forge a path for subsequent research by the community.

Type: Renewal
Title: "Predictions of Thermal Striping in Sodium Cooled Reactors"

Principal Investigator: Andrew Siegel, Argonne National Laboratory
Co-Investigators: Paul Fischer, Argonne National Laboratory
Dinesh Kaushik, Argonne National Laboratory
Aleksandr Obabko, Argonne National Laboratory
Won Sik Yang, Argonne National Laboratory

Scientific Discipline: Nuclear 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:
This project will use computer simulation to aid in the design optimization of a new generation of Advanced Recycle Reactors (ARR). These reactors will be used to greatly reduce the amount of spent fuel storage required by light water reactors. A critical issue in the design of sodium-cooled fast reactors is predicting the phenomenon of "thermal striping" —when partially mixed streams of sodium coolant expose structural materials to cyclic thermal stresses that cause fatigue and limit their lifetime. Thermal striping is particularly predominant in the outlet plenum, where the heated sodium enters as discrete jets with widely varying temperatures. Over the lifetime of the reactor, the temperatures of these jets vary according to changing fuel composition and control rod movements, and the reactor designer must account for the impact on upper plenum structures over the entire range of conditions. Traditionally, designers have relied on data from instrumented experiments, but this data is expensive and difficult to collect, and greatly limited in its spatial fidelity and adaptability to scope design space. For this reason computation has also been employed, but with reduced models and a level of incorporated empiricism that greatly limits predictability. This project will use INCITE resources to carry out the first detailed numerical experiments of thermal striping on realistic reactor geometries. The results can be directly used by U.S. ARR designers to create a more optimized design.

Type: Renewal
Title: "Predictive and Accurate Monte Carlo Based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems"

Principal Investigator: Thomas C. Schulthess, Swiss National Supercomputing Centre
Co-Investigators: Jerzy Bernholc, North Carolina State University
David Ceperley, University of Illinois–Urbana-Champaign
Markus Eisenbach, Oak Ridge National Laboratory
Mark Jarrell, Louisiana State University
Paul Kent, Oak Ridge National Laboratory
Alexandru Macridin, University of Cincinnati
Thomas Maier, Oak Ridge National Laboratory
Clare McCabe, Vanderbilt University
Lubos Mitas, North Carolina State University
G. Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Sciences

INCITE Allocation: **70,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (70,000,000 processor hours)

Research Summary:
Better electric grid technologies, high-density magnetic hard drives, and more efficient biofuel production require that we understand and optimize relevant materials. This project will perform simulations of Mott insulators, high-temperature superconductors, magnetic nanoparticles and select biomolecular systems that are key for these goals and will accelerate development of such technologies. Applying recent advances in Monte Carlo techniques, this project will push the envelope of computational science at the petascale in order to understand, predict, design, and exploit complex behavior that emerges at the nanoscale. Initial emphasis will be to break new ground in our understanding of transition metal oxide systems, where strong electronic correlations drive emergent behavior, such as high-temperature superconductivity in the cuprates. In the longer term, our simulations will lead to breakthroughs in nanoscale systems, such as nanomagnets and biomolecular systems with complex interactions, subject to temperature-driven fluctuations and entropic effects. Quantum Monte Carlo-based ab initio molecular dynamics simulations will provide new benchmarks for the development of empirical models, help validate the choice of functionals in Density Functional Theory-based simulations, and in the distant future, might even be directly integrated with the Wang-Landau scheme.

Type: New
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 profoundly new physical and chemical phenomena that arise at length scales intermediate between those of isolated molecules and bulk materials have been the subject of an explosion in nanoscience research in the past decade. These novel properties, which cannot be understood by simple extrapolation of either molecular or bulk properties into the nano regime (hence "non-scalable"), have been exploited for applications ranging from high-strength carbon nanotubes to highly active catalytic materials. In spite of these powerful and important developments, however, fundamental understanding of how nanoscale objects differ from their smaller or larger cousins (molecules and bulk materials, respectively) has been lacking. The only means of performing reliable electronic structure analyses of nanosystems is to perform explicit electronic structure calculations of these nanometer-sized objects, calculations that have been prohibitively costly to date.

In this work, we will combine novel, highly parallelizable electronic structure (Density Functional Theory) codes with the hardware available through the INCITE program to provide unprecedented insights into the evolution of the electronic and chemical properties of metal particles across the nanoscale regime. This analysis will, firstly, determine the critical size at which nanoparticles of various geometries become truly metallic (bulk-like) in their electronic structures; this is a fundamental, unresolved question in nanoscience. Additionally, by coupling this electronic analysis to related calculations of the surface catalytic properties of platinum and gold nanoparticles, we will answer the longstanding question of whether changes in nanoparticles' electronic properties with size can account for the remarkably high catalytic activities that have been experimentally observed in nanoparticles with diameters of 2-4 nm. Taken together, our combined electronic and catalytic analyses will provide novel physical insights into the nano regime and, as such, will open up significant new possibilities for the manipulation and selection of nanoparticles for groundbreaking technological applications.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

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

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **25,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (25,000,000 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. Historically, docking has a mixed success rate. 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 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.

We propose to utilize the advanced Blue Gene/P systems to conduct 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. We will also conduct the first large-scale study of the computationally intensive FEP/MD-GCMC methodology for estimation of free binding energy. Finally, in collaboration with the Center for Structural Genomics of Infectious Diseases, we will conduct 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 important validation step necessary to evaluate the predictive power of biomolecular simulations. This project will utilize a fully functioning computational pipeline that was developed under a director's discretionary allocation.

Type: New
Title: "Quantum Simulations of Nanostructural Materials for Renewable Energy Applications"

Principal Investigator: Giulia Galli, University of California, Davis
Co-Investigators: Francois Gygi, University of California, Davis

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **1,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (1,000,000 processor hours)

Research Summary:
We propose to use quantum simulation techniques to predict structural, electronic and optical properties affecting the scientific design of nanostructured materials to use for photovoltaic and thermoelectric applications. We focus on the study of surfaces and interfaces at the nanoscale, in particular assembly, embedding, and solvation of semiconductor nanoparticles, with the goal of providing a microscopic description of nanostructured materials in realistic environments, directly comparable with experimental conditions. We address two major problems:

(i) simulate systems using realistic structural models of integrated nanostructures, e.g. quantum dots embedded in solid matrices; and

(ii) provide an efficient and accurate description of excited state properties of nanostructures, beyond standard Density Functional Theory, so as to understand and predict electronic properties involved in calculations of absorption spectra and catalytic processes (in the case of photovoltaics) and electrical and thermal conductivity and Seebeck coefficient (in the case of thermoelectric materials).

Type: New
Title: "Research into the Systematics of Type Ia Supernovae"

Principal Investigator: Alan Calder, Stony Brook University
Co-Investigators: Aaron Jackson, Stony Brook University
Dean Townsley, University of Arizona

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
The mechanism by which a compact star known as a white dwarf explodes in a type Ia supernova explosion remains a conundrum. Observations indicate these bright events form a very homogeneous class, which allows their use as "standard candles" (distance indicators) for cosmological studies. Observational campaigns aimed at measuring the expansion history of the Universe, including the NASA/DOE Joint Dark Energy Mission, assume that these events have only a small intrinsic scatter, yet the mechanism is incompletely understood and concerns remain about scatter and systematic biases. The goal of this proposed study is a better understanding of type Ia supernovae, particularly a theoretical explanation for systematic trends and an assessment of intrinsic scatter. Demonstrating a robust mechanism for type Ia supernova explosions has the potential to significantly advance scientific knowledge in the disciplines of cosmology and galactic chemical evolution by providing a theoretical understanding that will better constrain uncertainty and thus improve the results obtained from studies utilizing type Ia supernovae as distance indicators.

This proposal will allow the investigators to meet this goal by performing the most realistic multidimensional simulations of these complex events ever undertaken. The simulations will assume the explosion paradigm of thermonuclear runaway occurring in a massive C/O white dwarf, and will incorporate advanced flame and dynamic ash models developed by the investigators and collaborators. The simulations are targeted at understanding the relationship between the first sparks that ignite the supernova flame, the turbulent flow field in which these sparks ignite, and the turbulence-enhanced deflagration that ensues. This relationship is critical to how much the star expands before being incinerated, what material is produced in the supernova, and the brightness of the resulting visual display. The study will pay particular attention to the role of state-of-the-art models for the sub-grid scale interaction between turbulence and flame. We will directly compare how modeled features in lower resolution simulations compare with resolved features at higher resolution, and contrast competing models for unresolved behavior.

Type: New
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:
High-end computing systems such as those being deployed at the Leadership Computing Facilities (LCF) consist of tens or hundreds of thousands of processors, terabytes of memory, exotic high-speed networks, and petabytes of storage. As hardware complexity sky-rockets in LCF 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. We propose studying four different classes of system software: Message Passing Libraries; Parallel I/O; Data Visualization; and Operating System.

Collaborators will use time on the platforms to understand and solve problems that occur at scale. The project team will leverage their connections with software development groups both in the DOE's Scientific Discovery through Advanced Computing and in the larger community to most effectively address challenges. Through rigorous experimentation, analysis, and design cycles, we 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: "Scalable System Software Research for Extreme-Scale Computing"

Principal Investigator: Ron Oldfield, Sandia National Laboratories
Co-Investigators: Ronald Brightwell, Sandia National Laboratories
Kurt Ferreira, Sandia National Laboratories
Suzanne Kelly, Sandia National Laboratories
James Laros, Sandia National Laboratories
Kevin Pedretti, Sandia National Laboratories
Rolf Reisen, Sandia National Laboratories

Scientific Discipline: Computer Science

INCITE Allocation: **5,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (5,000,000 processor hours)

Research Summary:
Over the last two decades, Sandia National Laboratories has been a leader in system software research for extreme-scale supercomputing systems. The lab's pioneering work on lightweight operating system research, starting with Sunmos, then Puma, Cougar, Catamount, and now Kitten, established lightweight kernels as the gold standard for extreme-scale systems and had a significant influence on vendor solutions such as IBM's compute-node kernel and Cray's compute-node Linux. In addition, Sandia's work on message passing, lightweight storage, power efficiency and utilization, and operating-system noise are all key contributors to the success of high-performance computing (HPC) systems today.

The goal of this project is to leverage the platforms provided by the Office of Science Leadership Computing Facilities (LCFs) to continue its efforts to improve system software for extreme-scale systems. In particular, this effort will use LCF systems to investigate scalability issues for research in lightweight operating systems, resilience, input/output, power efficiency, and debugging. The results of these efforts promise to significantly advance the state of the art for system software on the next generation of HPC systems.

Type: Renewal
Title: "Sculpting Biological Membranes by Proteins"

Principal Investigator: Klaus Schulten, University of Illinois–Urbana-Champaign

Scientific Discipline: Biological Sciences

INCITE Allocation: **25,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (25,000,000 processor hours)

Research Summary:
Cells in the human body organize their functions through intricately shaped lipid membranes forming organelles like the nucleus or endoplasmic reticulum. Biologists are now discovering how these organelles are shaped bottom-up from the smallest cell components, proteins, with advanced computing furnishing the key microscopic views bridging the molecular and cellular scales. Living cells are characterized by intricately curved internal membranes forming organelles, which facilitate cellular processes. During the cell lifecycle, the curvature is sculpted by proteins that act on a nanometer scale but through concerted action produce cell-scale (i.e., micrometer) shapes.

The shaping of cells is one of the most fascinating and "hottest" areas in modern cell biology and has been the subject of a series of prominent recent publications. The mystery to be resolved is that overall cellular shapes are induced by molecular (i.e., local) events that naturally need to be concerted in a self-organized manner to produce cell-scale shapes. The computational "microscope" driven by today's most advanced hardware and software, jointly with new conceptual approaches to multiscale simulation, promises to make not only a genuine contribution to the field of cellular membrane morphology, but will become a decisive instrument for resolving the magnificent geometrical and functional organization of entire living cells.

Type: New
Title: "Sequencing DNA using MspA"

Principal Investigator: Aleksei Aksimentiev, University of Illinois–Urbana-Champaign

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
High-throughput technology for sequencing DNA has already provided invaluable information about the organization of the human genome. However, the high cost of whole-genome sequencing limits widespread use of this method in basic research and personal medicine. This project investigates a novel method of sequencing a DNA molecule using MspA, a pore-forming protein of *Mycobacterium smegmatis*. In this method, a negatively charged DNA molecule is driven through a single MspA pore suspended in a lipid bilayer membrane by a voltage difference imposed across the membrane. As a DNA strand passes through the pore, the sequence of its nucleotides is detected by measuring the transient reductions of the ionic current through the pore.

Several problems need to be resolved for this approach to be useful in practice. Foremost, improvements in the architecture of the MspA protein will be required to slow the translocation of single DNA strands so that the sequence of the entire DNA molecule can be determined in one measurement. Furthermore, to enable rational engineering of the protein, the physical mechanism of the ionic current detection must be elucidated. Such work could take many years if done using purely experimental approaches. Computer simulations can play a unique role in designing MspA for sequencing applications as they can directly relate the conformation of the DNA and the protein to the ionic current and the DNA translocation velocity, something no experimental method can accomplish. Thus, this project presents a once-in-a-lifetime opportunity to radically advance the key technology in the emerging era of personal medicine through high-performance computing.

Type: Renewal
Title: "Simulation of Global Cloudiness"

Principal Investigator: David Randall, Colorado State University
Co-Investigators: Ross Heikes, Colorado State University
John Helly, San Diego Supercomputer Center
Bruce Palmer, Pacific Northwest National Laboratory
Karen Schuchardt, Pacific Northwest National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **3,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (3,000,000 processor hours)

Research Summary:
Global atmospheric modeling has been an active area of research for about 40 years. The models are very successful when they are applied to numerical weather prediction, but their application to the simulation of climate change has been more problematic. The most severe difficulties are associated with our inability to realistically simulate the interactions between cloud systems and the global-scale circulation of the atmosphere.

Better climate models can be made by reducing the horizontal grid spacing to a few kilometers or less, but for the next several decades limitations of computer power will prevent this. Better models can also be made by improving the parametric representations, or "parameterizations," of important unresolved processes, but at present our limited understanding prevents this. We are proposing a third approach that is just barely feasible with current supercomputers, and which appears to be within reach of our current understanding.

Our research will create and nurture a major and radically new activity in the field of global atmospheric modeling that will enable rapid progress toward more realistic climate-change simulations. Our long-term goals are to achieve a much better understanding of the role of clouds in climate variability, to develop and demonstrate new ways to compare high-resolution observations with global model results by creating stronger and more fruitful interactions between global modelers on the one hand and cloud-scale observers and cloud modelers on the other, to enable major and rapid progress toward reliable simulations of anthropogenic climate change, and to contribute to the development of improved weather forecasts from the operational centers.

Type: New
Title: "Simulation of 'High' Reynolds Number Turbulent Boundary Layers"

Principal Investigator: Robert Moser, University of Texas at Austin
Co-Investigators: Javier Jimenez, Universidad Politechnica de Madrid

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:

Nearly 20% of world energy consumption is expended on transportation, in which vehicles move through air or water, or fluids are transported through pipes and ducts. The energy expenditure is needed due to the interaction between solid surfaces (of vehicles or pipes) and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. Thus at least 20% of world energy consumption is necessitated by turbulence and the energy it dissipates. Since much of the drag in these flows is due to the turbulent skin friction much of this energy consumption is caused directly by wall-bounded turbulent shear layers.

Engineering design, particularly to manipulate turbulent wall layers, is hindered by our poor understanding of the physics of flow turbulence. The goal of the proposed simulations is to address this poor understanding for the canonical zero-pressure-gradient (ZPG) turbulent boundary layer, the prototype for turbulent boundary layers, such as those on vehicles.

A spatially-growing turbulent boundary layer with zero-pressure-gradient over a flat plate has already been simulated in a large box, at Reynolds numbers up to $Re_\theta = 2000$. This has provided preliminary insights on the difference between internal (pipes or channels) and external (boundary layers) turbulent flows, particularly on the effect of large-scale intermittency on the turbulent structure of the outer edge of the turbulent region. Final clarification of the physics requires increasing the Reynolds number by a factor of 2-3, because the range of scales of the present simulation is insufficient to differentiate between inner and outer scales. Previous experience with turbulent channel simulations ($Re_\tau = 550 - 2000$) is that the minimum Re needed for reasonably definite conclusions is about 1800, while the present boundary layer has a maximum $Re_\tau = 700$. The aim of this proposal is to increase the Reynolds number by about a factor of 2.5, to achieve the same flow quality as in the channels. Boundary layers are the primary interface between vehicles (e.g. airplane, boats) and the medium in which they move. Their physical understanding is not only an intellectual challenge, but a prerequisite for better vehicle design.

Type: Renewal
Title: "Simulation and Modeling of Membranes Interactions with Unstructured Proteins and Computational Design of Membrane Channels for Absorption of Specified Ions"

Principal Investigator: Igor Tsigelny, University of California, San Diego
Co-Investigators: Mark Miller, University of California, San Diego

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
Unstructured protein samples many different conformations in solution and undergoes rapid interconversion among these various forms in water. By simulating the various conformations sampled by protein in solution, we can further investigate the likelihood of its forming multimeric complexes in solution and on the surface of a phospholipid bilayer; possible further aggregation toward porelike structures with the following penetration to the membrane; and perforation of the bilayer. Such pore creation would cause flow of selected ions to and out of the cell. For biomedical purposes it would be needed to stop the entire process of aggregation/pore formation. This can stop progression of various diseases (Parkinson's, Alzheimer's, Huntington's, prion, etc). The process of pore formation can also be modified for specific needs. For environmental purposes the pores could be constructed in a way that they will permit flow to the cell of the selected ions only (for example radionuclides).

This project will focus on the development of a program package for modeling of aggregation and membrane pore formation by unstructured proteins leading to neurodegenerative diseases (Parkinson, Alzheimer, Huntington, prion, etc.) and methods to stop aggregation; and on computational engineering of microorganisms with molecular pores that will absorb the specified ions and compounds (for example radionuclides).

Type: New
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: **45,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (45,000,000 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. 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 energetics campaign begins in the late summer of 2009, and continues into 2010. Here, sub-scale targets, designed to emulate laser-plasma interactions (LPI) in ignition targets, will be fielded. The ignition campaign begins in earnest in 2010, where ignition will be achieved using 1.2-1.8 MJ of 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 proposes to perform 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, inertial fusion, as well as on the fundamental science of LPI.

Type: Renewal
Title: "Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models"

Principal Investigator: Don Lamb, University of Chicago ASC FLASH Center
Co-Investigators: Anshu Dubey, University of Chicago ASC FLASH Center
Robert Fisher, University of Chicago ASC FLASH Center
Nathan Hearn, University of Chicago ASC FLASH Center
George Jordan, University of Chicago ASC FLASH Center
Michael Papka, University of Chicago ASC FLASH Center
Katherine Riley, University of Chicago ASC FLASH Center
Dean Townsley, University of Chicago ASC FLASH Center
Klaus Weide, University of Chicago ASC FLASH Center

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **70,000,000 Processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (70,000,000 Processor hours)

Research Summary:
Type Ia supernovae (SNe Ia) are thought to be white dwarf stars in binary systems that explode due to a thermonuclear runaway. Observations using SNe Ia as "standard candles" revealed that the expansion rate of the universe is accelerating and led to the discovery of dark energy. Understanding dark energy ranks among the most compelling problems in all of physical science. Most scientists in the field believe that using SNe Ia to determine the properties of dark energy will require accurate simulations of SNe Ia and quantification of the uncertainties in the predictions made by these simulations.

Two major challenges face numerical astrophysicists in the Type Ia supernova (SN Ia) field: (1) buoyancy-driven turbulent nuclear combustion, which is a key physical process in SNe Ia, is not fully understood; and (2) very few simulations of the four current models of SN Ia have been done, making it difficult to determine which of these models is favored by observations, and even more, what values of the many parameters specifying these models are consistent with observations. We propose to use this INCITE award to meet both of these challenges. This validation program will advance the SN Ia field dramatically, leading to a deeper understanding of these models and quantification of the uncertainties in the predictions made by them. It also has the potential to impact the design of the instruments, the scientific observing strategy, and the analysis and interpretation of data for JDEM and other large projects whose goals are to determine the properties of dark energy.

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

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

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
Plasma is a ubiquitous form of matter in the universe. It is nearly always found to be magnetized and turbulent. One must understand this behavior to interpret a large body of astronomical observations. Examples include turbulence in the interstellar medium, which is stirred by violent events like supernova explosions; turbulence in accretion flows around stars and compact objects; and turbulence in the solar wind streaming outward from our Sun. Whether one is expressly interested in the turbulent fluctuations themselves or not, many observations are strongly affected by the amplitude of the fluctuations as a function of wave number and frequency.

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. The project will 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
Co-Investigators: Johan Larsson, Stanford University
Eric Johnson, Stanford University
Parviz Moin, Stanford University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **12,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (12,000,000 processor hours)

Research Summary:
We propose to conduct direct numerical simulations of the Richtmyer-Meshkov instability and the ensuing turbulent multi-material mixing. The proposed INCITE allocation will allow us to study the fundamental physics governing this phenomenon, in particular the mechanisms at play in turbulent multi-material mixing in high-speed accelerated flows. This study will use a novel solution-adaptive numerical framework that scales well and that will enable science discovery through high-performance computing.

The 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, the perturbations grow; if the incoming shock is strong enough or if the interface is sufficiently perturbed, the instability evolves into a turbulent mixing region. Though the early evolution of the hydrodynamic instability has been studied extensively, few investigations of the turbulent multimaterial mixing that occurs at late time have been carried out for two main reasons: inadequacy of the numerical algorithms, unknown and possibility prohibitive computational cost. With the proposed allocation, we will be able to address important questions in fluid mechanics, as we will be able to carry out, for the first time, direct numerical simulations of the turbulent multimaterial mixing generated after the RMI. Based on our estimates, we will be able to resolve the viscous dissipation in this flow, so that we are confidently representing the physics of this problem accurately. The turbulence statistics that we will compile will provide invaluable data to answer fundamental questions: 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? What controls how long does the flow depend on the initial conditions? 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?

Type: New
Title: "Ultrascale Simulation of Basin-Scale CO_2 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: **18,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (18,000,000 processor hours)

Research Summary:
This project brings petascale computing resources to bear on current environmental issues. These include sequestration of greenhouse gases such as CO_2 in deep geologic formations to mitigate global warming, and migration of radionuclides from highly contaminated DOE legacy sites from World War II and the Cold War. By applying petascale computing to extreme-scale problems involving CO_2 sequestration in large geologic basins, the project will investigate the effects on drinking water aquifers of displacing deep formation water brines with large volumes of CO_2. In addition, it will apply petascale resources to uranium migration at the Hanford 300 Area in Washington State. New data for stratigraphy, heterogeneity, and chemical processes are becoming available as part of an ongoing DOE/Integrated Field Research Challenge (IFRC) project focused on the 300 Area, and to the project will incorporate this information into a larger revised site model. To minimize effects of inland boundary conditions on the local flow field, it will extend the domain away from the Columbia River, increasing domain size and requiring increased resources over the current 4,096 processor-cores currently being used. Finally, at the Oak Ridge IFRC site, the project will assist members of the ORNL IFRC project in constructing a watershed-scale groundwater model with refined resolution using high-performance computing for sites at the Oak Ridge Reservation. This model will integrate multiple processes at multiple scales into the model to investigate both the influence of process interactions at small scales on the fate and transport of contaminants in the field, and the scale dependency of controlling parameters such as dispersivity, attenuation, mass transfer, and reaction rates. The calculations planned for this allocation will be the largest groundwater simulations ever carried out to date.

Type: New
Title: "Unbalanced Magnetohydrodynamic Turbulence"

Principal Investigator: Stanislav Boldyrev, University of Wisconsin-Madison
Co-Investigators: Fausto Cattaneo, University of Chicago
Joann Mason, University of Chicago
Jean Perez, University of Wisconsin-Madison

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
Most of the baryonic matter in the Universe, including intergalactic and galactic media, the interstellar medium, interiors of planets and stars, is magnetized and turbulent. Magnetohydrodynamics (MHD) provides the simplest framework for describing magnetic plasma turbulence. In a stark contrast with usual hydrodynamic turbulence, which tends to forget the large-scale conditions and become progressively more isotropic at smaller scales, MHD turbulence develops strong local anisotropy and imbalance as the scale of the fluctuations decreases. Moreover, magnetic plasma turbulence in nature and in the laboratory is typically strongly anisotropic and unbalanced already at large scales as it is guided by strong external fields (e.g., fusion devices) or driven by localized sources (e.g., solar wind, supernovae explosions).

Recently, certain new effects related to anisotropy and imbalance have been discovered and several thought-provoking phenomenological theories have been put forward. However, these theories produce conflicting predictions, and the currently available numerical simulations are not able to resolve the contradictions either. The goal of this project is to conduct a comprehensive numerical study of anisotropic unbalanced (or cross-helical) magnetohydrodynamical turbulence with very high, currently unmatched resolution. A specially designed set of numerical simulations with varying Reynolds numbers and varying degrees of imbalance will be performed, which will allow one to resolve the controversies among current theories, develop the correct picture of strong MHD turbulence, and provide valuable data for comparison with astrophysical models and laboratory experiments.

Type: New
Title: "Uncertainty Quantification for Three-Dimensional Reactor Assembly Simulations"

Principal Investigator: Thomas Evans, Oak Ridge National Laboratory
Co-Investigators: Kevin Clarno, Oak Ridge National Laboratory
Matthew Jessee, Oak Ridge National Laboratory
Wayne Joubert, Oak Ridge National Laboratory
Scott Mosher, Oak Ridge National Laboratory
Bradley Rearden, Oak Ridge National Laboratory

Scientific Discipline: Energy Technologies: Nuclear Energy

INCITE Allocation: **8,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (8,000,000 processor hours)

Research Summary:
The performance of nuclear fuel in boiling water reactors (BWRs) is strongly dependent on the power distribution within a nuclear fuel bundle. Vendor software, as is typical in the nuclear industry, provides pin-averaged power distribution data on a 6-inch axial grid, which is much too large to be able to determine the within-pin power distribution near the control blades, before and after withdrawal. Recent work with the Denovo three-dimensional, discrete ordinates transport code has demonstrated the ability to model the power distribution for this problem on a ¼-inch axial grid with a 6 mil (0.006 inch) radial (*x, y*) mesh (using 60,000 cores on the Cray XT5 at ORNL). Therefore, it is clear that the solution is within reach.

However, the problem is not simply single-physics radiation transport. The effective macroscopic nuclear cross-sections, which are used in a radiation transport solver, are linearly dependent upon the density of the materials. Before we proceed to develop a coupled thermal-fluid-dynamics and radiation transport solver, it is necessary to evaluate the fidelity of each that is required. Evaluating the sensitivity of the radiation transport solution to the spatial resolution of the coolant density would guide the software development of a coupled physics solver by determining the "fidelity" requirements of the thermal-fluid-dynamics solver.

Uncertainty quantification is one of the most important, and least implemented, topics in computational science. As numerical algorithms and high-performance computing architectures have become more advanced and powerful, the ability to model complex physical phenomena has grown to the point where computer models are often used in place of experiment.

Type: New
Title: "Understanding the Ultimate Battery Chemistry: Rechargeable Lithium/Air"

Principal Investigator: Jack Wells, Oak Ridge National Laboratory
Co-Investigators: Edoardo Apra, Oak Ridge National Laboratory
Ray Bair, Argonne National Laboratory
Peter Cummings, Vanderbilt University
Alessandro Curioni, IBM Zurich Research Laboratory
Paul Kent, Oak Ridge National Laboratory
Teodoro Laino, IBM Zurich Research Laboratory
William Shelton, Oak Ridge National Laboratory
Winfried Wilcke, IBM Almaden Research Center
Ye Xu, Oak Ridge National Laboratory

Scientific Discipline: Energy Technologies: Energy Storage

INCITE Allocation: **24,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (12,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (12,000,000 processor hours)

Research Summary:
A rechargeable Lithium/Air battery can potentially store ten times the energy of a Lithium/Ion battery of the same weight. But realizing this enormous potential is a very challenging scientific problem. However, we expect that with petascale supercomputer simulation the key scientific problems can be understood and substantial advances made during the next few years. Therefore, a research coalition is being established between IBM Research, Universities and DOE labs to understand the chemistry and demonstrate a working prototype of such a battery.

Lithium/Air cells consist of an anode (ideally Lithium metal), an electrolyte - which can be either aprotic or aqueous - and the air cathode. We will focus on aprotic systems, as these are known to be rechargeable and have the highest energy storage density. It has been demonstrated that it is possible, at least at low electrical current densities, to reverse this process and convert the Li2O2 back into Lithium metal. This exciting proof-of-principle work still presents very big scientific challenges before one can be confident that practical propulsion batteries can be based on the Li/Air system. The most important ones are to realize a high percentage of the theoretical energy density, to improve electrical efficiency of recharging, to increase the number of times the battery can be cycled, to limit the negative effects of moisture in the air, and to improve the power density. To this end, our research project is focused on understanding (1) the mechanisms of Lithium/Air cell discharge and recharge reactions, (2) the role and selection of catalyst and cathode surface properties, (3) the solubility of lithium ion and lithium oxides and optimization of electrolyte, and (4) the reactions occurring at the electrode-electrolyte interface.

Type: Renewal
Title: "Validation of Plasma Microturbulence Simulations for Finite-Beta Fusion Experiments"

Principal Investigator: William Nevins, Lawrence Livermore National Laboratory
Co-Investigators: Jeff Candy, General Atomics
William Dorland, University of Maryland
Darin Ernst, Massachusetts Institute of Technology
Greg Hammett, Princeton Plasma Physics Laboratory
Christopher Holland, University of California–San Diego
David Mikkelsen, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
Plasma microturbulence, the dominant mechanism for the loss of heat from tokamak fusion reactors, will determine the fusion gain that can be achieved in the international ITER reactor. While plasma microturbulence has been studied since the 1960s, the magnetic fusion community has yet to develop a complete predictive understanding of the turbulent transport of heat, momentum, and particles across magnetic surfaces. The development of such a predictive understanding has been identified as a major goal for the U.S. fusion program, and achieving it requires the validation of high-fidelity plasma microturbulence codes. This proposal is to validate the three most advanced plasma microturbulence codes in the U.S. program (GYRO, GS2, and GEM) against transport and fluctuation data from the three large U.S. tokamak experiments (DIII-D, C-MOD, and NSTX), and employ these codes to predict transport losses in ITER. This code validation effort directly addresses the U.S. fusion program goal of developing a predictive understanding of plasma transport, and supports the mission of the Center for the Study of Plasma Microturbulence.

Type: Renewal
Title: "Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas"

Principal Investigator: Patrick Diamond, University of California–San Diego and Howard Hughes Medical Institute

Co-Investigators: C.S. Chang, New York University
Stephane Ethier, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Zhihong Lin, University of California–Irvine

Scientific Discipline: Plasma Physics

INCITE Allocation: **35,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (35,000,000 processor hours)

Research Summary:
Predicting and controlling turbulent transport are among the most important and challenging scientific issues facing the international ITER fusion reactor. Three topics in particular address the need to understand nonlinear plasma dynamics and self-organization in complex tokamak geometry: cascades and propagation in collisionless trapped electron mode (CTEM) turbulence, turbulent transport of toroidal momentum and the origins of intrinsic rotation, and global kinetic simulation of toroidal Alfven instability. All three topics are exceedingly challenging, requiring multiscale, non-local processes of turbulence self-organization. All three address problems that are highly relevant to ITER and are of interest in the broader arena of physics. Nonlinear simulations using a gyrokinetic toroidal code (GTC) for tokamak core and a gyrokinetic particle-in-cell code (XGC) for tokamak edge will address these important scientific issues and cross-benchmark. The predictive capability of the GTC and XGC dynamical models will be validated by comparing simulation results with the largest fusion experiments in the United States (DIII-D, ALCATOR C-MOD, and NSTX tokamaks). These simulations will advance the frontier of computational sciences in the areas of data management, statistical analysis, and advanced visualization.

Type: Renewal
Title: "The Via Lactea Project: A Glimpse into the Invisible World of Dark Matter"

Principal Investigator: Piero Madau, University of California–Santa Cruz
Co-Investigators: Juerg Diemand, University of California–Santa Cruz
Michael Kuhlen, Institute for Advanced Study
Ben Moore, University of Zurich
Doug Potter, University of Zurich
Joachim Stadel, University of Zurich
Marcel Zemp, University Michigan

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **5,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (5,000,000 processor hours)

Research Summary:
The universe is dominated by a mysterious, weakly interacting particle that accounts for five-sixths of its total matter content. These "dark matter" particles are known to gravitationally hold galaxies like our own Milky Way together. Revealing their nature and their clumping properties is one of the fundamental challenges of particle physics and cosmology. The Via Lactea Project has produced the most detailed picture of the galactic dark matter halo to date and provides new clues to the formation and assembly history of the Milky Way.

The main goal of this project is to perform the largest simulation ever of the assembly of the dark matter cloud that is known to hold our galaxy together. This project will take the next crucial step toward resolving the small-scale structure of galactic dark matter and refine the predictions for indirect dark matter detection experiments. The unprecedented cosmological simulation described here will advance the field dramatically and provide definite answers to the following questions: What is the ab undance and distribution of dark matter substructure within the solar circle? Can nearby clumps of dark matter be detected by the Fermi Large Area Space Telescope? What is the antimatter and neutrino flux at Earth from dark matter annihilation? Do simulations reproduce the dense cores observed in dark matter-dominated Milky Way dwarf satellites? Does the rich mass distribution predicted by the cold dark matter paradigm agree with the recent explosion of data probing galactic phase-space substructure?